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SPIKE: A COMPUTER MODEL FOR THE H₂(D₂) + F₂ PULSED CHEMICAL LAS--ETC(U)

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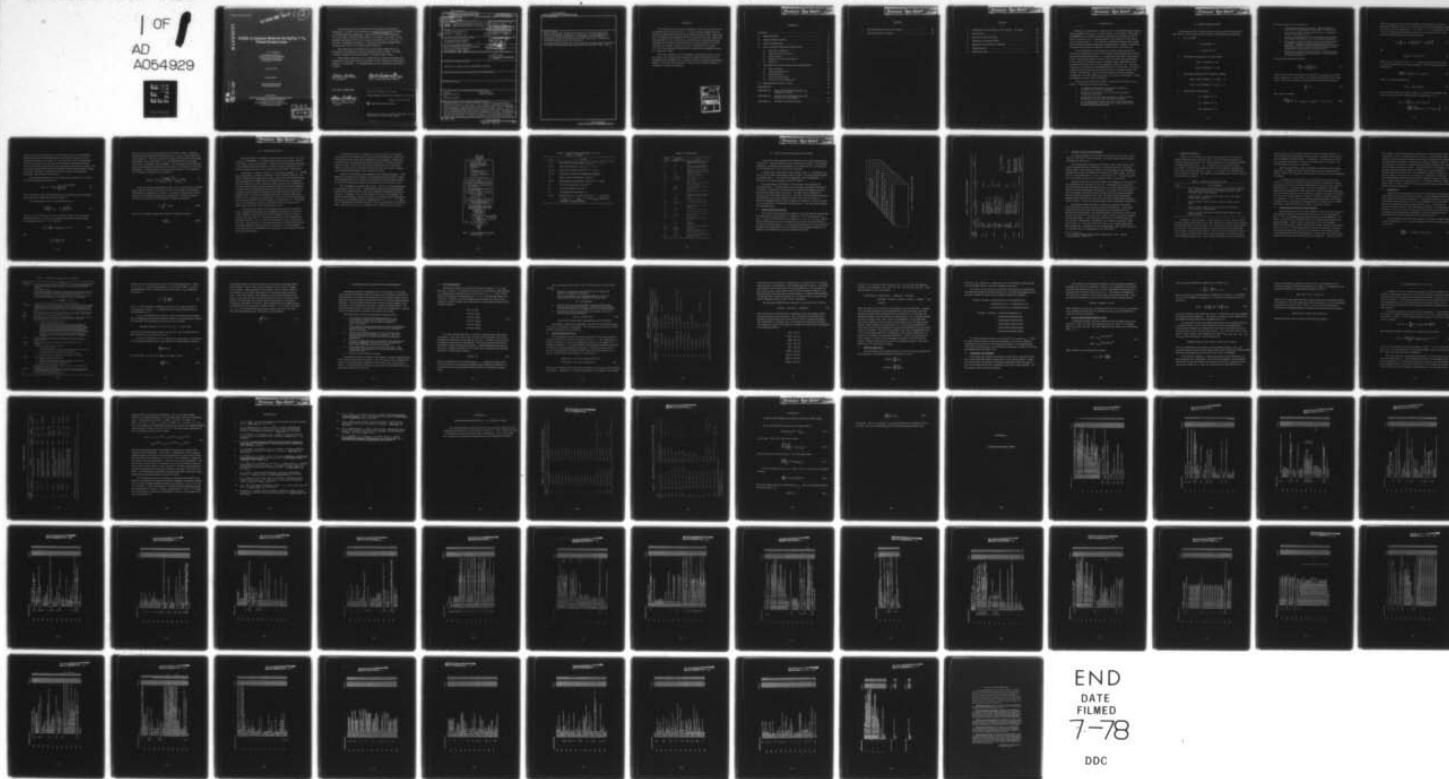
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SPIKE: A Computer Model for the $H_2(D_2) + F_2$ Pulsed Chemical Laser

J. J. T. HOUGH

Aerophysics Laboratory
The Ivan A. Getting Laboratories
The Aerospace Corporation
El Segundo, Calif. 90245

14 April 1978

Interim Report

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This technical report has been reviewed and is approved for publication. Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

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| 20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A comprehensive rate equation model for a pulsed laser pumped by the H ₂ (D ₂)-F ₂ reaction is described. This computer simulation incorporates up to 216 kinetic reactions to describe the laser medium, which is assumed to be homogeneous and contained in a Fabry-Perot optical cavity. The first fifteen vibrational-rotational P-branch transitions from each of the lowest ten vibrational bands are monitored for possible laser action. The distinctive features incorporated in this model include: (1) the elimination of the gain-equals-loss assumption, so that it is possible to predict cavity transients | | |

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20. ABSTRACT (Continued)

and to observe gain-intensity interactions; (2) a detailed model of the Lorentz broadening, including V, J dependence, as well as distinction between various perturbing species; (3) multiquantum HF(DF) self-deactivation, which in the HF case was found important to achieve good agreement between theory and experiment.

Comparisons of the prediction of this model with several small-scale experiments have indicated generally good agreement (typically within ~20%).



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PREFACE

The preliminary work in the development of this code was carried out at Michigan State University with R. L. Kerber and was supported by the Division of Engineering Research of the College of Engineering. Subsequent work, including the incorporation of the D_2-F_2 kinetics and the comparisons with experiments, was carried out at The Aerospace Corporation and was supported by the Defense Advanced Research Projects Agency, the Naval Sea Systems Command, and the Air Force Weapons Laboratory under U.S. Air Force Space and Missile Systems Organization (SAMSO) Contract No. F04701-77-C-0078.

This code originally was not intended for distribution; hence, it may not contain some convenience measures that might be desirable from the standpoint of the unfamiliar user. Sufficient detail is provided in this report, however, such that, with some effort, the user will be able to modify the program for his specific purposes.

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I. INTRODUCTION

SPIKE, a comprehensive computer model of the HF(DF) pulsed chemical laser pumped by the $H_2(D_2) + F_2$ chain reaction, is described. This model incorporates up to 216 kinetic reactions and takes into detailed account the effects of pressure line-broadening based on the results of a recent survey of the literature (Ref. 1). The method of computation utilized in this model did not require the gain-equals-loss assumption and is capable of predicting transients and relaxation oscillations within the laser cavity (Ref. 2).

Recent comparisons of the predictions of this model with several small-scale pulsed H_2-F_2 laser (~ 25 -cm gain length) experiments revealed generally good agreement (Ref. 2). Comparisons with larger scale experiments (~ 100 -cm gain length), however, have not shown as good agreement in the prediction of absolute energy, although relative performance with parameter variations still showed comparable results (Ref. 3). This lack of agreement is indicative of possible deficiencies in the model. It has been suggested that such phenomena as photoionization, photodissociation, and medium nonuniformity, which have been neglected in typical modeling calculations, may have significant impact on the larger scale lasers. These possibilities are still under investigation.

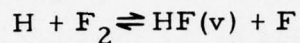
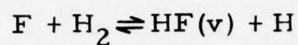
Several recent requests for SPIKE, reflect the need for this "users guide." The objectives in this report are:

1. To explain the theories from which the calculations executed in the code are formulated.
2. To present in systematic form the formal and logical structures of the code.
3. To describe the procedures necessary in order to obtain information from this code with minimal lag time.
4. To provide sufficient detail such that, with some preparation, modifications to the code can be made so that it can be tailored to particular needs.

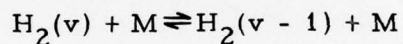
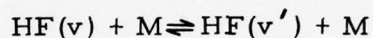
II. MODEL FORMULATION

The formulation of the chemical laser computer model is described in this section. The reactions used to represent the chemical processes are:

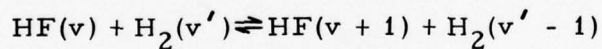
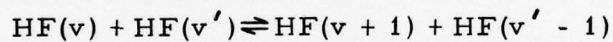
1. $H_2 + F_2$ chain



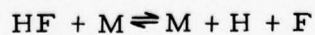
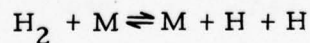
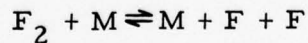
2. Vibrational-translational (VT) deactivation



3. Vibrational-vibrational (VV) quantum exchange



4. Dissociation-recombination



The major features in the models are:

1. The dominant kinetic processes are represented by the reaction system suggested by Cohen (Ref. 4) (Table A-1).
2. The reacting mixture is homogeneous and is contained in a Fabry-Perot laser cavity.
3. The rotational populations for each vibrational level have a Boltzmann distribution at the translational temperature.
4. All possible transitions within a band are assumed to have low initial intensities that grow if the gain rises above threshold. Lasing is always assumed to be in the P-branch. Initial intensity levels can be selected individually or set proportional to the spontaneous emission rate.
5. Initiation is modeled by the introduction of a finite concentration of F atoms into the gas mixture, or through the use of a flash-lamp option.

The chemical reactions are written

$$\sum_i \alpha_{ri} N_i \xrightleftharpoons[k_{-r}]{k_r} \sum_i \beta_{ri} N_i \quad (1)$$

where N_i is the molar concentration of species i , α_{ri} and β_{ri} are stoichiometric coefficients, and k_r and k_{-r} are forward and backward rate coefficients. The rate of change of concentration for nonlasing molecules is

$$\frac{dN_i}{dt} = X_i \quad (2a)$$

and, for HF molecules,

$$\frac{dN_{\text{HF}(v, J)}}{dt} = X_i + X_{\text{rad}}(v, J) - X_{\text{rad}}(v - 1, J_L) + A(v, J) \quad (2b)$$

where the X_{rad} terms are rates of change in concentration as a result of lasing into and out of level (v, J) . The lower-level rotational quantum numbers are J and J_L for the transitions $v + 1 \rightarrow v$ and $v \rightarrow v - 1$, respectively. The net rate of spontaneous emission into level (v, J) is given by $A(v, J)$. The chemical reactions yield a concentration change

$$X_i = \sum_r (\beta_{ri} - \alpha_{ri}) \left(k_{r+} \prod_j N_j^{\alpha_{rj}} - k_{-r} \prod_j N_j^{\beta_{rj}} \right) \quad (3)$$

and

$$X_{\text{rad}}(v, J) = g(v, J) f(v, J) \quad (4)$$

where $g(v, J)$ is the gain on the $v + 1 \rightarrow v$ transition with lower level J and $f(v, J)$ is the lasing flux on the same transition. The rate equation for the lasing flux is

$$\frac{df(v, J)}{dt} = c \left(\frac{L}{\ell} \right) [g(v, J) - \alpha_{\text{thr}}] f(v, J) \quad (5)$$

where c is the speed of light and

$$\alpha_{\text{thr}} = - \frac{1}{2L} \ln(R_O R_L) \quad (6)$$

where L is the length of the active medium, ℓ is the mirror spacing, and R_O and R_L are the mirror reflectivities. The gain (Ref. 5) is

$$g(v, J) = \frac{hN_A}{4\pi} \omega_c(v, J) \phi(v, J) B(v, J) \times \left[\left(\frac{2J+1}{2J-1} \right) N_{\text{HF}(v+1, J-1)} - N_{\text{HF}(v, J)} \right] \quad (7)$$

where $\omega_c(v, J)$ is the wave number of the transition, $B(v, J)$ is the Einstein isotropic absorption coefficient based on the intensity, and $\phi(v, J)$ is the Voigt profile at line center (Ref. 6). The first term of Eq. (5) determines the rate of increase in the intensity of the radiation field within the laser cavity; the second term gives the rate energy that is lost from the cavity. The lost energy includes that extracted through the output coupler as laser output, as well as real losses resulting from such mechanisms as absorption, scattering, and extraneous reflections.

A Boltzmann distribution at the translational temperature (T) is taken for the rotational populations; hence,

$$N_{HF}(v, J) = N_{HF}(v) \left(\frac{2J+1}{Q_r^v(T)} \right) e^{-hcE_J^v/kT} \quad (8)$$

where the values of the rotational partition function $Q_r^v(T)$ and the rotational energy E_J^v are computed from Mann et al. (Ref. 7).

The energy equation for a constant density gas is

$$\frac{dT}{dt} \sum_i N_i C_{v_i} = -P_L - \sum_i \frac{dN_i}{dt} H_i \quad (9)$$

where C_{v_i} is the molar specific heat at constant volume, H_i is the molar enthalpy of species i , and P_L is the output lasing power per unit volume. The output power in the $v+1 \rightarrow v$ band is

$$P_{Lv}(t) = \sum_J hc N_A \alpha_{thr} \omega_c(v, J) f(v, J) \quad (10a)$$

and

$$P_L(t) = \sum_v P_{Lv}(t) \quad (10b)$$

where the only cavity loss is assumed to be the laser output. In making comparisons with experimental measurements, however, real losses must be accounted for. One way to do this is to assume that fraction of the output attributable to the "total reflector" R_L (as distinguished from the output coupler R_o) corresponds to cavity losses. The transmissivity of the mirror (R_L) may be adjusted to approximate cavity losses resulting from scattering, transmission, and absorption at various optical surfaces. The useful fraction of the total output power is then (Ref. 6)

$$P_{\text{useful}} = \frac{P_{\text{total}}(1 - R_o)}{[1 + (R_o/R_L)^{1/2}][1 - (R_o/R_L)^{1/2}]} \quad (11)$$

From the numerical integration of Eqs. (2), (5), and (9) by the modified Adams-Moulten method of Gear (Ref. 8), the time evolution of the species concentrations, temperature, pressure, the gain on all transitions, and the intensities on all lasing transitions are determined. The laser energy extracted in each band is then determined by integrating the power

$$E_v = \int_0^{t_c} P_{Lv} dt \quad (12a)$$

where t_c is the length of laser pulse and the total pulse energy is

$$E = \sum_v E_v \quad (12b)$$

III. CODE DESCRIPTION

The broad features of SPIKE are described in this section. The code is written in FORTRAN. A complete listing of the main program and the subroutines is given in Appendix C. In addition to the explanations provided in this and the subsequent sections, extensive comment statements are included throughout the body of the listing to provide further clarification.

The program consists of a main (or controlling), program, i.e., SPIKE, and six subroutines: INPUT1, LORENTZ, GAIN, DIFSUB, DIFFUN, and RATE. SPIKE obtains input data by calling subroutine INPUT1 and initiates such computational variables as concentration, photon flux, temperature and time; defines the cavity conditions; obtains reaction rate constants and necessary spectroscopic and thermodynamic data from data files; updates the pressure line-broadening parameters through the use of the subroutine LORENTZ; and provides the program control parameters that direct the program flow, as well as the integration process. Subroutine (function) GAIN is used to compute the medium gain of the laser for any given allowed vibrational-rotational P-branch transition by means of Eq. (7). The photon fluxes corresponding to the seven transitions within each band with the highest gain are monitored for possible laser action.

Time progression within the model proceeds along the integration steps. Numerical integration is accomplished through the use of the subroutine DIFSUB, which utilizes the modified Adams-Moulten technique presented by Gear (Ref. 8). Derivatives required for the integration are computed from Eqs. (2), (5), and (8) and obtained by means of subroutine DIFFUN. Laser initiation by electrical discharge (or flash photolysis) may be modeled through a flash-lamp option contained in the main program, which provides a time-dependent F-atom production rate based on the input power (intensity) profile.

Substantial savings in computation time and computer core storage requirements were obtained with the present code formulation, wherein the rate equations were input as an integral part of the program, and the rate coefficients were precomputed and stored on disk for retrieval during program execution. In the event that minor modifications to the rates are desired, rather than re-creating the entire rate file, these minor changes are accomplished through the use of subroutine RATE.

Figure 1 is a schematic flow diagram of the computer program. This figure is an overview of the chain of commands and decisions used to obtain the integrated values of the species concentrations within the laser medium, as well as the laser power density and temperature as a function of time.

The variables and symbols used in Fig. 1 and in the computer program are defined in Tables 1 and 2. Bookkeeping limitations and computational practicability demand that the many time-dependent variables be grouped in an array. In addition, since the dimension of an array is changeable, the model has the flexibility to alter the number of variables under consideration. The array is two dimensional and is designated $Y(I, J)$, $J = 1, \dots, N$, where $Y(1, J)$ represents the variable in question, N is the total number of such variables, and $Y(I, J)$ and $I > 1$, are related to the $(I - 1)$ th derivatives of $Y(1, J)$.

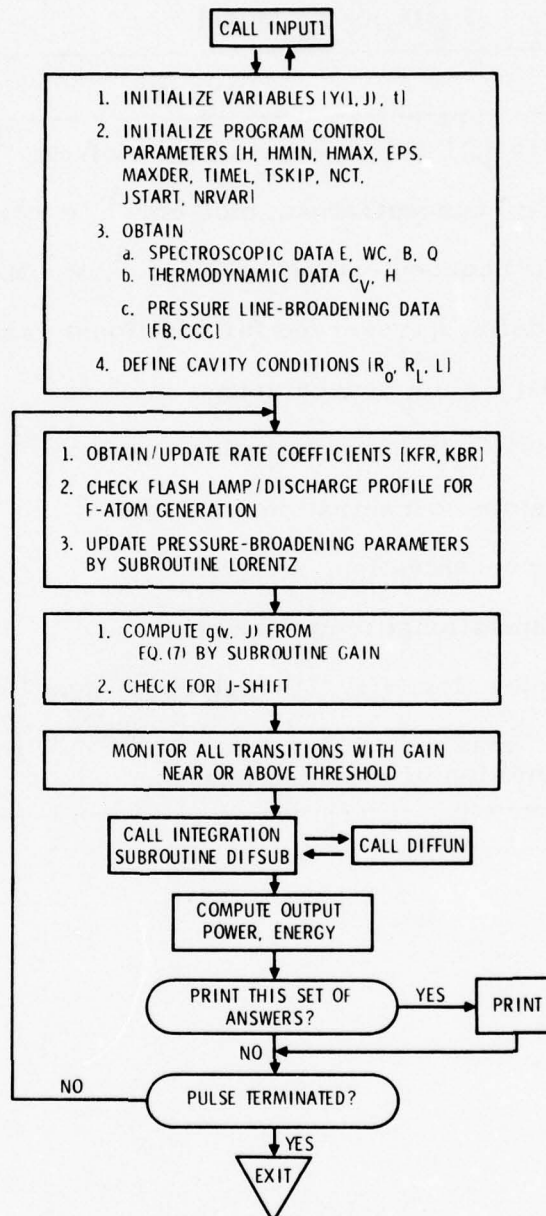


Fig. 1. Pulsed HF(DF) Chemical Laser Model

Table 1. Identification of Variables $Y(1, N)$ in
 $H_2(D_2) + F_2$ Model

| N | $Y(1, N)$ |
|-------|---|
| 1-9 | $HF(v)[DF(v)]$ concentration, mol-cm^{-3} , $v = N-1$ |
| 10-11 | $DF(v)$ concentration, mol-cm^{-3} , $v = N-1$ |
| 12-14 | $N_2(v)$ concentration, mol-cm^{-3} , $v = N-12$ |
| 15-16 | Undefined, reserved for additional variables |
| 17 | $H(D)$ - atom concentration, mol-cm^{-3} |
| 18-20 | $H_2(v)[D_2(v)]$ concentration, mol-cm^{-3} , $v = N-18$ |
| 21 | F -atom concentration, mol-cm^{-3} |
| 22 | F_2 concentration, mol-cm^{-3} |
| 23 | Translational temperature, K |
| 24-79 | Photon flux, $f(v, J)$, $\text{mol-cm}^{-2}\text{-sec}^{-1}$, $v = (N-17)/7 $, $J = J_{\max}^v - 4, \dots, J_{\max}^v + 2$, where J_{\max}^v indicates the transition of maximum gain. |

Table 2. Nomenclature

| Symbol in Text | Symbol in Computer Program | Definition |
|---|----------------------------|--|
| A(v, J) | A(V, J) | Einstein isotropic coefficient for spontaneous emission, 1/molecule-sec |
| B(v, J) | B(V, J) | Einstein isotropic intensity absorption coefficient, cm ² /molecule-J-sec |
| c | C | Speed of light, 2.997925×10^{10} cm/sec |
| C _{V_i} ^v | CVI | Molar specific heat at constant volume of species i, cal/mol-K |
| E _J ^v | E(V, J) | Rotational energy of state V, J, cm ⁻¹ |
| f(v, J) | FLUX(V, J) | Photon flux, mol-cm ⁻² -sec ⁻¹ |
| g(v, J) | ALPHA(V, J) | Gain of transition (v + 1, J - 1) → (v, J), cm ⁻¹ |
| h | - | Planck's constant, 6.6256×10^{-34} J-sec |
| h | - | Specific enthalpy, kcal/g |
| H _i | EHPYI | Molar enthalpy of species i, kcal/mol |
| I | CRRNT | Discharge current, A |
| k | K | Boltzmann's constant, 1.38054×10^{-23} J-K ⁻¹ |
| k _r , k _{-r} | KFR, KBR | Forward and backward rate constants, in terms of moles, centimeters, and seconds |
| L | LNTH | Length of active medium, cm |
| N _i | Y(I, I) | Concentration of species i, mol-cm ⁻³ |
| dN _i /dt | DERV1Y(I) | Time derivative of N _i , mol-cm ⁻³ -sec ⁻¹ |
| N _A | NA | Avogadro's number, 6.02252×10^{23} molecules-mol ⁻¹ |
| P _L | POWER | Power density of laser output, W-cm ⁻³ |
| P _I | PIN | Power input from initiation, W-cm ⁻³ |
| Q _r ^v | Q(V, T) | Rotational partition function for level v |
| R _O R _L | RO, RL | Mirror reflectivities |
| R | R | Universal gas constant, 1.98725 cal-mol ⁻¹ -K ⁻¹ |
| t | T | Time, sec |
| T | Y(I, 23) | Temperature, K |
| α _{ri} , β _{ri} | - | Stoichiometric coefficients of reaction r |
| α _{thr} | THGAIN | Threshold gain, cm ⁻¹ |
| φ(v, J) | PHI(V, J) | Normalized line profile of transition (v + 1, J - 1) → (v, J), cm |
| τ _R | TAU(V, J) | Rotational relaxation time constant, sec |
| ω _c (v, J) | WC(V, J) | Wave number of transition (v + 1, J - 1) → (v, J), cm ⁻¹ |

IV. BASIC INSTRUCTIONS FOR USING SPIKE

The common input preparations needed for most runs are discussed in this section. The input parameters are classified as follows: (1) initial gas conditions, (2) optical cavity parameters, (3) output control, (4) integration control parameters, and (5) initiation mechanism.

A sample set of input data cards is shown in Fig. 2. The proper location for these cards is immediately after the end-of-record card that follows the program decks. This format corresponds to that of NAMELIST. A summary of the input variables is given in Table 3.

The input data are divided into seven groups; each group has an identifying name. The data stream for each group is initiated by the sign \$ in Column 2, followed by the group name (no blank must appear between \$ and the group name) and then the data. The data must be separated by commas, and terminated by another \$. However, the data within each group can be listed in any order and may extend to more than one record. It should be emphasized that no data can appear in Column 1 of any one record, as it is ignored by the NAMELIST READ operation. The seven data streams are described below.

A. INITIAL GAS CONDITIONS

The initial concentrations of the species in the gas mixture are provided through the data stream SPECIES. In addition to the reacting species F_2 , H_2 , F, and H, several diluents are modeled, i.e., He, Ar, N_2 , SF_6 , and O_2 . These concentrations may be provided in any units (but must be consistent) or simply as relative ratios. An initial $HF(0)$ population may also be entered. Pressure of the gas mixture in Torr (PRESS) and initial gas temperature in degrees kelvin (TEMP) are input by the data stream GAS.


```

      EOF
$FLASH2 FLASH = 0., 0., 0., 1., 36=0$
$FLASH1 Z1 = .012, Z2 = .5, WPHOTO = 0.$
NVAR = 83$
$STEPS DELTA = 4E-10, HMIN=1.E-15, HMAX=.5E-9, EPS=1.E-1, JSTART=0,
KBS =2$
$OUTPUT1 TIMEL=10.E-6, TCHECK=3.E-6, POFF=1.E-1, TSKIP= 1E-6, IPEEK=0,
$CAVITY R0 = .52, RL = .9, LINTH = 100., LRATIO = 1., FLUX = 1.E-14$
$GAS PRESS = 800., TEMP = 300.$
AR = .37, H = 0.$
$SPECIES H2=.03, F2=.06, F=.0006, O2=.0., HE=.54, N2=.0., SF6=.0., HF=.0.,
      EOR

```

Fig. 2. Sample Input Data for SPIKE

Table 3. Summary of Input Variables

| Group Name | Variable | Definition | Units | Comments |
|------------|---|--|---|--|
| SPECIES | H ₂ , F ₂ , F, H, He, Ar, N ₂ , O ₂ , HF, SF ₆ | Species concentrations | Arbitrary | |
| GAS | PRESS TEMP | Total gas pressure Gas temperature | Torr Kelvin | |
| CAVITY | R0 RL LNTH LRATIO | Output coupler reflectivity Mirror reflectivity Medium gain length Ratio of gain length to mirror separation | - - cm - | |
| | FLUX | Initial photon flux | mol/cm ² -sec | |
| OUTPUT1 | TIMEL TCHECK | Upper limit of integration Check for pulse termination at t > TCHECK | sec sec | |
| | POFF TSKIP IPEEK | Power density at termination Time between prints Controls limited print option | W/cm ³ sec - | IPEEK = { 0, Full print 1, Limited print 1 ≤ KBS ≤ 5 |
| STEPS | KBS DELTA HMIN HMAX EPS JSTART NVAR | Printout format selector Initial step size Minimum step size Maximum step size Error test constant Input indicator Number of integration variables | - sec sec sec sec - | See Table 5 for more complete information |
| FLASH1 | Z1 Z2 WPHOTO | Peak flash lamp output Defined by Eq. (14) Average energy of absorbed photon | mol/cm ³ cm ⁻¹ | |
| FLASH2 | FLASH(2,20) | I(1), t(1), I(2), t(2), ..., I(20), t(20) | I = nondimensional t = sec | FLASH1 and FLASH2. Data are not needed if flash option not used. It is not required to use all 40 elements in this array. |

B. OPTICAL-CAVITY PARAMETERS

The input parameters for the laser optical cavity are R0, RL, LNTH, LRATIO, and FLUX. These quantities, contained in data stream CAVITY, are defined in this section.

The optical cavity is assumed to be Fabry-Perot, with mirror reflectivities denoted by R0 and RL and given in decimal fractions. R0 is the output coupler, and only that fraction of the total radiant energy that passes through this mirror is included in the calculation of laser output. Note that the "0" in the symbol R0 is a "zero," not the letter "O." The gain length of the active medium is given by the variable LNTH in centimeters.

LRATIO is the ratio of the gain length to the separation of the mirrors, corresponding to the L/l factor in Eq. (5). This parameter accounts for the intervals during which the photons traverse regions between the mirrors, which are neither amplifying nor absorbing. The larger the "null" region, the fewer passes each photon makes through the active medium during the photon residence time within the cavity. This phenomenon reduces the amplification potential of the cavity and can result in appreciable reduction in laser output. It has been observed experimentally at Sandia Laboratories.¹

All possible transitions within a band are assumed to have initial intensity levels that grow if the gain rises above threshold. These initial intensity levels can be selected individually or set proportional to the spontaneous emission rate. Our standard practice has been to set all initial intensity levels at 10^{-14} mol/cm²-sec, which is done by setting the variable FLUX to this value. Test cases where this value was varied by as much as $\times 10^3$ have indicated the calculations to be relatively insensitive to this number (Ref. 2). The value of FLUX is set to zero to make small signal gain calculations. (Alternatively, the threshold gain value can be increased to any large number by adjusting R0, RL, and LNTH.)

¹J. B. Moreno, Sandia Laboratories, Albuquerque, N.M., private communication, April 1977.

C. OUTPUT CONTROL

TSKIP, KBS, and IPEEK are three input parameters that control the quantity and form of the computer output. As the calculation progresses, pertinent data are printed at time intervals specified by the parameter TSKIP (seconds) beginning at time $t = 0$. A final print is also obtained at pulse termination. Contents of the printed output are controlled by the parameter KBS, which may have values of $1 \leq \text{KBS} \leq 5$. The larger the value selected, the more print is obtained. The outputs corresponding to the various values of KBS are shown in Table 4.

Table 4. Definition of Parameter KBS

| KBS | Printed Output |
|-----|---|
| 1 | Time, laser power, laser energy, gas temperature, species concentrations, total number of integration steps to reach this time, and the last step size. |
| 2 | Output of KBS = 1 plus the photon flux, power, and energy of each laser transition. |
| 3 | Output of KBS = 2 plus the gain of each transition at this time. |
| 4 | Output of KBS = 3 plus the self-broadening coefficients $\gamma(v, J)$ and other linewidth data. |
| 5 | Output of KBS = 4 plus rate coefficients and reaction rates for all reactions. |

In addition to printed output, an array (XXX) is written, which contains the laser power, laser energy, time, gas temperature, species concentrations, and gain and power of each transition. At each print interval, XXX is copied onto Tape 13. The parameter KKK is incremented each time to keep track of the number of times XXX is copied. At the end of the calculation, Tape 13 may be saved, either for later use in a plotting program or for a brief scan of the calculated results (e.g., this file may be quickly retrieved and studied

on an interactive terminal while the main output is waiting to print). If only the abbreviated output data contained in XXX is needed, the main print may be skipped by setting IPEEK = 1 (otherwise, it should be set to zero). The resulting output will be two prints corresponding to the initial ($t = 0$) and final (pulse termination) conditions.

The input data TSKIP, KBS, and IPEEK are punched in data stream OUTPUT1. In addition to these, this data stream also contains the data TIMEL, POFF, and TCHECK, which determine the point at which computation is stopped.

Termination of the calculation occurs with the onset of one of two events: (1) integration reaches an imposed time limit specified by TIMEL (seconds) or (2) the power density drops below some preset level, given by $\text{POFF}(\text{W}/\text{cm}^3)$. In the latter case, to avoid terminating the calculation during the developing phase of the laser power, this terminating mechanism does not become operative until an interval, TCHECK (seconds), has elapsed. The user must provide values for TIMEL, TCHECK, and POFF as part of the input data. In the case of a small-signal-gain calculation, where power remains at zero, termination of computations is controlled only by TIMEL. The value of TCHECK should be set larger than that of TIMEL.

D. INTEGRATION CONTROL PARAMETERS

Numerical integration of the rate equations within the present model is accomplished utilizing a modified Adams-Moulten technique presented in Ref. 8. The corresponding integration subroutine is called DIFSUB. The reader is referred to the original reference for details regarding this integration package. Under ordinary circumstances, only the variables NVAR(=N), DELTA(=H), HMIN, HMAX, EPS, YMAX, KFLAG, and JSTART will be of concern. NVAR represents the number of integration variables contained in the program, DELTA is the step size to be attempted on the next integration step, HMIN and HMAX are, respectively, the minimum and maximum step sizes that will be used for the integration. EPS is an error

test constant, which represents the maximum error (estimate) that can be tolerated on a step; it is expressed as a "fraction" of the maximum value (YMAX) of each integration variable (Y) seen up to this point in the integration. The user also has the option of adjusting the values of YMAX to influence the step sizes. KFLAG is an output flag from DIFSUB that gives the result of the previous integration attempt. A KFLAG value of +1 indicates a successful step, whereas a negative value corresponds to an unsuccessful one. JSTART defines the action on the next integration attempt: to repeat the previous step, to continue with a new step, or to indicate the first step. A more detailed description of these and other variables is given in Table 5; the contents of which are taken from Ref. 8. The value of DELTA, HMIN, HMAX, EPS, JSTART, and NVAR must be provided through the data stream STEPS to make a calculation.

E. INITIATION

Initiation of the chemical reactions is either through an instantaneous introduction of F atoms into the gas mixture or a time-dependent dissociation of F₂ molecules by a flash-lamp option. If the flash-lamp option is selected, input values for the parameters Z1, Z2, and WPHOTO must be provided, along with a flash-lamp output intensity profile (I vs t). These data are entered by means of data streams FLASH1 and FLASH2. For instantaneous initiation, on the other hand, the user need only provide an initial F-atom concentration in the data stream SPECIES, neglecting the data streams associated with the flash-lamp option FLASH1 and FLASH2.

The formulation of the flash-lamp option in the present model is similar to that in RESALE (Ref. 6). The rate of dissociation of the absorbing species n_a is given by

$$\left(\frac{dn_a}{dt}\right)_{fl} = -Z_1 I(t) [1 - \exp(-Z_2 n_a)] \quad (13)$$

Table 5. Definition of Parameters in DIFSUB

| Parameter | Definition |
|-----------|---|
| N = NVAR | The number of first-order differential equations. N may be decreased on later calls if the number of active equations reduces, but it must not be increased without calling with JSTART = 0. |
| T | The independent variable. |
| Y | An 8 by N array containing the dependent variables and their scaled derivatives. Y(J + 1, I) contains the J-th derivative of Y(I) scaled by H**J/factorial(J) where H is the current step size. Only Y(1, I) need be provided by the calling program on the first entry. If it is desired to interpolate to non-mesh points, these values can be used. If the current step size is H and the value at T + E is needed, form S = E/H, and then compute $Y(I) (T + E) = \sum_{J=0}^{NQ} Y(J + 1, I) * S**J$ |
| SAVE | A block of at least 12*N floating point locations used by the subroutines. |
| H = DELTA | The step size to be attempted on the next step. H may be adjusted up or down by the program in order to achieve an economical integration. However, if the H provided by the user does not cause a larger error than requested, it will be used. To save computer time, the user is advised to use a fairly small step for the first call. It will be automatically increased later. |
| HMIN | The minimum step size that will be used for the integration. Note that on starting this must be much smaller than the average H expected since a first-order method is used initially. |
| HMAX | The maximum size to which the step will be increased. |
| EPS | The error test constant. Single-step error estimates divided by YMAX(I) must be less than this in the Euclidean norm. The step and/or order is adjusted to achieve this. |
| MF | The method indicator. The following are allowed: <ol style="list-style-type: none"> 0 An Adams predictor corrector is used. 1 A multi-step method suitable for stiff systems is used. It will also work for non-stiff systems. However, the user must provide a subroutine PEDERV which evaluates the partial derivatives of the differential equations with respect to the Y's. This is done by call PEDERV(T, Y, PW, M). PW is an N by N array which must be set to the partial of the I-th equation with respect to the J dependent variable in PW(I, J). PW is actually stored in an M by M array where M is the value of N used on the first call to this program. 2 The same as Case 1, except that this subroutine computes the partial derivatives by numerical differencing of the derivatives. Hence PEDERV is not called. |
| YMAX | An array of N locations which contains the maximum of each Y seen so far. It should normally be set to 1 in each component before the first entry (See the description of EPS.) |
| ERROR | An array of N elements which contains the estimated one-step error in each component. |
| KFLAG | A completion code with the following meanings: <ol style="list-style-type: none"> +1 The step was successful. -1 The step was taken with H = HMIN, but the requested error was not achieved. -2 The maximum order specified was found to be too large. -3 Corrector convergence could not be achieved for H .GT. HMIN. -4 The requested error is smaller than can be handled for this problem. |
| JSTART | An input indicator with the following meanings: <ol style="list-style-type: none"> -1 Repeat the last step with a new H. 0 Perform the first step. The first step must be done with this value of JSTART so that the subroutine can initialize itself. +1 Take a new step continuing from the last. JSTART is set to NQ, the current order of the method at exit. NQ is also the order of the maximum derivative available. |
| MAXDER | The maximum derivative that should be used in the method. Since the order is equal to the highest derivative used, this restricts the order. It must be less than 8 or 7 for Adams or stiff methods, respectively. |
| PW | A block of at least N**2 floating point locations. |

where n_a is the concentration (mol/cm^3) of the absorbing species. Values for Z_1 , Z_2 , ω_v , and a flash-lamp profile $I(t)$ must be provided. Z_1 is the peak flash-lamp output in moles per unit volume of gas. Z_2 is defined by the relation

$$Z_2 = \frac{\alpha_v \ell}{n_a} \frac{\text{cm}^3}{\text{mole}} \quad (14)$$

where α_v is the absorption coefficient of species n_a in a gas container of mean geometric length ℓ . ω_v (WPHOTO) is the average energy of the absorbed photon in cm^{-1} .

Z_1 , Z_2 , and WPHOTO are input by means of the data stream FLASH1, and the flash-lamp output intensity profile is input by the data stream FLASH2. The format for the flash-lamp intensity profile is as follows:

$$\text{\$FLASH2 FLASH} = I(1), t(1), I(2), t(2), \dots, I(20), t(20)$$

where $I(k)$ is the flash output intensity at time $t(k)$. $I(k)$ is nondimensional, and its peak value is normalized to unity.

As shown in Appendix B, for an optically thin gas mixture, the initiation level through photodissociation of F_2 reduces to the approximate expression

$$\frac{[F]}{[F_2]} \cong 2 Z_1 Z_2 \quad (15)$$

For such cases, Z_2 can be set equal to one-half to obtain

$$\frac{[F]}{[F_2]} \approx Z_1 \quad (16)$$

This approximation provides an alternative technique for simulating flash-lamp initiation, which, under certain conditions, may be easier to apply. As an example, suppose parametric calculations must be made in which it is desired to vary the flash-lamp profile but maintain the same initiation level. With this technique, after setting Z_1 to the desired initiation level, and Z_2 to one-half, all that is needed for each new run is a new flash-lamp profile. This procedure is certainly easier than using Eq. (13) directly. It should be remembered, however, that in applying the above approximation the flash profile is normalized in a different sense. In the "exact" treatment i.e., Eq. (13), the peak flash value is set to unity, whereas, in the optically thin approximation case, the profile is normalized by

$$\int_0^{\infty} I(t) dt = 1 \quad (17)$$

V. CHANGING RATE EQUATIONS AND COEFFICIENTS

Substantial savings in computation time and computer core storage requirements were obtained with the present code formulation, wherein the rate equations were input as an integral part of the program and the rate coefficients were precomputed and stored on disk for retrieval during program execution. The drawback of this economy measure is that changes in rate equations or rate coefficients can require a rather significant effort. The economy gained, however, is believed to justify this inconvenience. The procedure for making these changes is described in this section.

The basic steps involved in making these changes follow:

1. New variables must be defined and initialized. The total number of integration variables is represented by the variable NVAR, which should be adjusted to reflect this change.
2. New reactions must be incorporated into subroutine DIFFUN, and the derivatives affected by these reactions updated to reflect the changes.
3. The thermodynamic properties of any new species introduced must be incorporated in the input data. The new species must also be considered in the gas temperature calculations.
4. Pressure-broadening effects contributed by the new species may not be negligible, in which case, the calculation for the Lorentz half-half width must be revised.
5. Rate modifications are made in the rate data files. Rate coefficients corresponding to new reactions must be added to these data files.
6. Format can be modified if desired.

A detailed description is given for the addition of oxygen-related kinetics to the code to illustrate the procedure. The reactions and rate constants utilized are essentially those compiled by Taylor et al. (Ref. 9) and given in Table 6. The deactivation of HF(v) by O₂ is taken to be similar to that by N₂, reduced by a factor of 3 (Ref. 10).

A. NEW VARIABLES

Several new species are introduced in these reactions: O , O_2 , H_2O , OH , HO_2 , and FO_2 . As indicated in Section III, the variables in this program are represented by elements in any array $Y(1, N)$, $N = 1, \dots, 100$. At this point, the locations corresponding to $N = 15, 16$, and 80 through 100 are unreserved. Therefore, the new variables may be assigned to any of these positions. In this example, the concentrations of these species will be represented as follows:

$$\begin{aligned} Y(1, 15) &= [O] \\ Y(1, 16) &= [O_2] \\ Y(1, 80) &= [OH] \\ Y(1, 81) &= [H_2O] \\ Y(1, 82) &= [FO_2] \\ Y(1, 83) &= [HO_2] \end{aligned} \tag{18}$$

For more efficient execution, it is best to keep the array dimension to a minimum. Thus, whereas a value of N up to 100 is possible, the present example was selected to occupy only up to $N = 83$. A smaller array may then be utilized for the program calculations. The input variable $NVAR$ was implemented to help accomplish this purpose. $NVAR$ designates the maximum size of the variable array that is to be used in the accompanying computation. Therefore, in the present situation,

$$NVAR = 83 \tag{19}$$

The new variables must also be initialized, i.e., assigned an initial value. A zero value will be automatically assigned unless otherwise instructed. It is assumed for the present purposes that only $Y(1, 16) = [O_2]$ has a nonzero value.

The following procedure may be used to introduce O_2 as a new input variable.

1. Expand the NAMELIST group SPECIES in the subroutine INPUT1 to include the variable O2.
2. Add O2 to GASSUM in the subroutine INPUT1. The fractional value of O2 is then computed by the statement:

$$O2 = O2/GASSUM$$

3. Add O2 to the common block GAS1, found in both the main program and subroutine INPUT1. Note that in this example, the variable name O2 was changed to RO2 in the main program.
4. Calculate the initial O_2 concentration (in moles/cm³) in the main program by the statement

$$Y(1, 16) = RO2*FCTR \quad (20)$$

where FCTR represents the appropriate conversion factor.

The location of these new statements, and others to be described below, are given in the listings in Appendix C. The changes described here are indicated in the listings by the symbol O_2 .

B. DIFFUN MODIFICATIONS

The no-oxygen version of the code incorporates 150 kinetic reactions, designated by the reaction numbers shown in Table A-1. The additional 14 reactions considered here will be designated by numbers 151 through 164, as indicated in Table 6. The variable NEQN (main program) should be set to 164 to reflect the increased number of reactions. For each of these reactions (K), the forward [RCTF(K)] and backward rates [RCTB(K)] must be computed. As an example, Reaction No. 151 is written as

$$\begin{aligned} RCTF(151) &= (Y(1, 15)**2)*M12*KFR(151) \\ RCTB(151) &= M12*Y(1, 16)*KBR(151) \end{aligned} \quad (21)$$

where it is recalled that Y(1, 15) and Y(1, 16) refer to the species concentrations of O and O_2 , respectively. KFR(151) and KBR(151) correspond to the forward

Table 6. Oxygen Kinetics

| Reaction No. | Reaction | Rate Constant (k) | |
|--------------|--|-------------------------------------|--|
| | | cm ³ /mol-sec | cm ⁶ /mol ² -sec |
| 151 | $O + O + M_{12} \xrightarrow{k} O_2 + M_{12}$ | $7.98 \times 10^{19} T^{-1.5}$ | $M_{12} = 2.82O, O_2$ |
| 152 | $O + O + M_{13} \xrightarrow{k} O_2 + M_{13}$ | $3.0 \times 10^{15} T^{-0.5}$ | $M_{13} = N_2$ |
| 153 | $H_2 + OH \xrightarrow{k} H_2O + H$ | $2.29 \times 10^{13} e^{-5200/RT}$ | |
| 154 | $H + O_2 \xrightarrow{k} OH + O$ | $2.71 \times 10^{14} e^{-16600/RT}$ | |
| 155 | $O + H_2 \xrightarrow{k} OH + H$ | $1.2 \times 10^{13} e^{-9000/RT}$ | |
| 156 | $H + O_2 + M_{14} \xrightarrow{k} HO_2 + M_{14}$ | $6.17 \times 10^{14} e^{1600/RT}$ | $M_{14} = M_3, O_2, 1.8 H_2, 1.8 H_2O$ |
| 157 | $H + OH + M_{15} \xrightarrow{k} H_2O + M_{15}$ | $4.72 \times 10^{16} e^{1850/RT}$ | $M_{15} = M_3, 5.1 H_2O$ |
| 158 | $H + O + M_3 \xrightarrow{k} OH + M_3$ | 6.17×10^{16} | |
| 159 | $OH + O + M_3 \xrightarrow{k} HO_2 + M_3$ | 3.6×10^{14} | |
| 160 | $H_2O + O \xrightarrow{k} 2OH$ | $4.22 \times 10^{13} e^{-18000/RT}$ | |
| 161 | $H + HO_2 \xrightarrow{k} 2OH$ | 1.81×10^{13} | |
| 162 | $H + HO_2 \xrightarrow{k} H_2 + O_2$ | 6×10^{12} | $M_3 = \text{all species}$ |
| 163 | $O + HO_2 \xrightarrow{k} OH + O_2$ | 6×10^{12} | |
| 164 | $F + O_2 + M_3 \xrightarrow{k} FO_2 + M_3$ | 1.8×10^{15} | |

and backward rate coefficients, respectively, of Reaction No. 151, and M12 represents the "concentration" of the catalytic species O and O₂. In the definition of M12, the concentration of O was multiplied by 2.82 to account for the larger reaction cross section with O as the third body compared to O₂. Note that M12, along with other catalytic species, is defined at the beginning of this subroutine, and that all these "M" variables must be converted from fixed to floating variables by the "REAL" statement.

The subroutine DIFFUN will compute the "net forward rate" RF(151)

$$RF(151) = RCTF(151) - RCTB(151) \quad (22)$$

which is then used to calculate the contributions to the derivatives of each species involved in these reactions. The contributions of Reaction Nos. 1 through 150 have already been accounted for in the no-oxygen formulation. The contributions of Reaction Nos. 151 through 164 remain to be included. The reader can easily verify that these reactions will affect the concentrations of the following species:

$$\begin{aligned} [O] &= Y(1, 15) \\ [O_2] &= Y(1, 16) \\ [H] &= Y(1, 17) \\ [H_2] &= Y(1, 18) \\ [F] &= Y(1, 21) \\ [OH] &= Y(1, 80) \\ [H_2O] &= Y(1, 81) \\ [FO_2] &= Y(1, 82) \\ [HO_2] &= Y(1, 83) \end{aligned} \quad (23)$$

Consider as an example atomic oxygen Y(1, 15). Its concentration depends directly on Reaction Nos. 151, 152, 154, 155, 158, 159, 160, and 163. Thus, the derivative of Y(1, 15) is written

$$\begin{aligned} \text{DERV1Y}(15) = & \text{DERV1Y}(15) - 2. * [\text{RF}(151) + \text{RF}(152)] \\ & + \text{RF}(154) - \text{RF}(155) - \text{RF}(158) - \text{RF}(159) - \text{RF}(160) \quad (24) \\ & - \text{RF}(163) \end{aligned}$$

where the first term accounts for contributions from Reaction Nos. 1 through 150, normally computed in preceding sections of the subroutine, and subsequent terms reflect the contributions from Reaction Nos. 151 through 164. Similar equations can be written for the other species. Two comments should be made in regard to Eq. (24). First, the leading term on the right-hand side of this equation is not necessary in this instance since its value is zero; however, this situation is not universal, e.g., in the case of DERV1Y(21). Thus, this term is always suggested to reduce the possibility of errors resulting from oversights. Second, it is possible to gain some computational economy by performing many of the calculations in this equation separately, as portions are repeated in subsequent statements. But the economy gained is at the expense of clarity of the individual rate equations (derivatives) and further complicates the process involved in changing reactions. The choice made here is to preserve that clarity.

C. ENERGY EQUATION

The contributions of the added species to the terms of the energy Eq. (9) are discussed. The following program variables are used.

$$\begin{aligned} \text{CVSUM} &= \sum_i N_i C_{V_i} \\ \text{ETHLPY} &= \sum_i \frac{dN_i}{dt} H_i \end{aligned}$$

where N_i , C_{V_i} , and H_i are, respectively, the concentration, molar specific heat at constant volume, and molar enthalpy of species i .

The values of C_{V_i} and H_i for each of the new species must be incorporated into the program data files (Section VI). The following statements may be used to update the values of the variables CVSUM and ETHLPY:

$$\begin{aligned} \text{CVSUM} = & \text{CVSUM} + \text{CVO}(\text{IT}) * \text{Y}(1, 15) + \text{CVO2}(\text{IT}) * \text{Y}(1, 16) \\ & + \text{CVOH}(\text{IT}) * \text{Y}(1, 80) + \text{CVH2O}(\text{IT}) * \text{Y}(1, 81) \\ & + \text{CVFO2}(\text{IT}) * \text{Y}(1, 82) + \text{CVHO2}(\text{IT}) * \text{Y}(1, 83) \end{aligned}$$

$$\begin{aligned} \text{ETHLPY} = & \text{ETHLPY} + \text{EHPYO}(\text{IT}) * \text{DERV1Y}(15) \\ & + \text{EPHYO2}(\text{IT}) * \text{DERV1Y}(16) \\ & + \text{EHPYOH}(\text{IT}) * \text{DERV1Y}(80) \\ & + \text{EHPYH2O}(\text{IT}) * \text{DERV1Y}(81) \\ & + \text{EHPYFO2}(\text{IT}) * \text{DERV1Y}(82) \\ & + \text{EHPYHO2}(\text{IT}) * \text{DERV1Y}(83) \end{aligned}$$

For dilute mixtures where O_2 concentrations are small (e.g., $\sim 0.5\%$), the effect of these species on the energy equation, as well as on pressure broadening (as discussed in the following paragraphs), is not appreciable. Under these circumstances, the modifications suggested in steps C and D may be neglected with very little error.

D. PRESSURE BROADENING

The foreign-gas broadened linewidth is calculated in subroutine GAIN. The Lorentz half-half width is represented by the variable LONTZ. Hence, the concentration and pressure-broadening coefficients of the new species must be incorporated into the computation of the value of this variable. For the present, only O_2 will be considered.

The collision-broadening characteristics of HF vibrational-rotational transitions by O_2 are not available. However, from published HCl pressure-broadened linewidth data (Ref. 11), it may be justifiably assumed that the O_2 characteristic is similar to that of H_2 or D_2 . The collision broadening of HF lines by O_2 is taken to be the same as H_2 in the present example. Thus, the following substitution is made in the statement that computes LONTZ:

$$H2SUM \rightarrow H2SUM + Y(1, 16)$$

where H2SUM is the total H_2 concentration and $Y(1, 16)$ is the O_2 concentration. This modification will result in a calculated Lorentz half-half width that accounts for the O_2 contribution.

E. RATE-COEFFICIENT MODIFICATION

As stated previously, the rate coefficients KFR and KBR used in equations such as Eq. (21) were precomputed and stored, either on a magnetic tape or on a disk, or both. The rate coefficients are taken to be of Arrhenius form, i.e.,

$$KFR = A_{fr} T^{B_{fr}} e^{E_{fr}/RT} \quad (25)$$

$$KBR = A_{br} T^{B_{br}} e^{E_{br}/RT}$$

KFR and KBR are connected by the relation

$$K_r = (RT)^v \frac{KFR}{KBR} \quad (26)$$

where K_r is the equilibrium constant of the reaction, and

$$\nu_r = \sum_i \nu_{ri} = \sum_i (\beta_{ri} - \alpha_{ri}) \quad (27)$$

where α_{ri} and β_{ri} are stoichiometric coefficients of reaction r , as defined in Eq. (1). The equilibrium constant K_r is a function of temperature only and is given by

$$\ln K_r = -\frac{1}{RT} \sum_i \nu_{ri} H_i + \frac{1}{R} \sum_i \nu_{ri} S_i \quad (28)$$

where H_i (cal/mole) and S_i (cal/mole-K) are, respectively, the molar enthalpy and molar entropy of species i . The values of H_i and S_i may be obtained from the JANAF thermodynamic data compilation (Ref. 12).

The generation of the rate coefficient data files is accomplished through a separate program, RATE. (Note that this is not the subroutine RATE.) This program computes, from input data, the forward and backward rate coefficients at 25-K intervals from 100 to 6000 K. The input data consist of one card for each reaction, which specifies the values of A_{fr} , B_{fr} , E_{fr} , A_{br} , B_{br} , and E_{br} in the order given. The format used is

FORMAT (E15.8, F9.5, E16.8, E15.8, F9.5, E16.8)

The rate coefficients are calculated in this program using Eq. (25). The generated data are copied onto the logical files TAPE7 (KBR) and TAPE12 (KFR), which are subsequently saved for future use by the model SPIKE.

Under certain conditions, a simpler procedure may be followed to obtain the needed rate coefficients. For the present example, the deactivation rate of HF(v) by O_2 was taken to be similar to that by N_2 , except that it was reduced by a factor of 3. Thus, the simulation of O_2 deactivation can be

easily accomplished by adding one-third of the O_2 concentration to the reactions that govern HF(v) deactivation by N_2 , which is accomplished in the subroutine DIFFUN by adjusting the definition of M11 to:

$$M11 = SF_6 + N_2 + 0.3*Y(1, 16)$$

where Y(1, 16) is the element in the variable array that corresponds to the O_2 concentration. The rate coefficients for HF deactivation by N_2 are presently computed in subroutine RATE. Thus, to ensure that this subroutine is exercised, the following statement should be inserted in the main program:

IF(RO2.GT.0.) CALL RATE (Y(1, 23))

where RO2 refers to the O_2 ratio in the initial gas mixture.

VI. DESCRIPTION OF DATA FILES

In addition to the rate coefficients contained in data files TAPE7 and TAPE12, the program must have access to spectroscopic and thermodynamic data that relate to the species in the reacting gas mixture. These are summarized in Table 7. The data are punched into data cards following the formats indicated in the table and input by means of program DATA, which reads the data and stores them at predetermined locations (indicated by the tape numbers).

Most of the data files in the table need no explanation. The rotational energies $E(v, J)$ and transitional wave numbers $WC(v, J)$ are computed from the data of Refs. 7 and 13. The rotational partition function can then be computed from the equation

$$Q(v, T) = 1 + \sum_{J=1}^{\infty} (2J + 1) \exp\left(-\frac{hc}{k} \frac{E(v, J)}{T}\right) \quad (29)$$

The Einstein absorption coefficient is computed from the relation

$$B(v, J) = \frac{16\pi^4 \times 10^{-7}}{3h^2 c} \left(\frac{2J}{2J + 1}\right) |\mathcal{M}_{v, J}^{v+1, J-1}|^2 \quad (30)$$

where the matrix elements for the transitions $\mathcal{M}_{v, J}^{v+1, J-1}$ are from Meredith (Ref. 14). The heat capacity (CV) and enthalpy (EHPY) data are obtained from the JANAF thermodynamic data compilation.

The role of pressure broadening in the pulsed HF chemical laser is discussed in detail in Ref. 1. Self-broadened linewidths are calculated by the use of the data CCC. Foreign-gas broadening is based on the experimental data compiled in Ref. 1 and stored in array FB. The coefficients contained in the array CCC were calculated by Meredith (Ref. 15) on the basis of the

Table 7. SPIKE Input Data

| Data Tape No. | Symbol | Definition | Format | Range | Units |
|------------------|---------------|--|--------|--|---|
| 1 | $E(v+1, J+1)$ | Rotational energy of state v, J | 5E14.5 | $v = 0, \dots, 9$ $J = 0, \dots, 30$ | cm^{-1} |
| 2 | $WC(v+1, J)$ | Wave number of transition ($v+2, J+1 \rightarrow v+1, J$) | 5E16.5 | $v = 0, \dots, 8$ $J = 1, \dots, 18$ | cm^{-1} |
| 3 | $B(v+1, J)$ | Einstein isotropic intensity absorption coefficient of transition ($v+2, J+1 \rightarrow v+1, J$) | 5E16.5 | $v = 0, \dots, 8$ $J = 1, \dots, 18$ | $\text{cm}^2 \text{mol}^{-1} \text{J}^{-1} \text{sec}^{-1}$ |
| 4 | $Q(v+1, T+1)$ | Rotational partition function for level v at temperature $T \times 100 \text{ K}$ | 5E16.5 | $v = 0, \dots, 8$ $T = (0, \dots, 60) \times 100 \text{ K}$ | |
| 8 ^a | $CV_i(T)$ | Molar heat capacity at constant volume of species i ($i = \text{F}, \text{F}_2, \text{N}_2, \text{SF}_6, \text{H}_2, \text{HF}$) at temperature $T \times 100 \text{ K}$ | 5F16.5 | $T = (1, \dots, 17) \times 100 \text{ K}$ | cal/mol-K |
| 9 ^a | $EHPY_i(T)$ | Molar enthalpy of species i ($i = \text{H}, \text{H}_2, \text{F}, \text{F}_2, \text{HF}$) at temperature $T \times 100 \text{ K}$ | 5F16.5 | $T = (1, \dots, 17) \times 100 \text{ K}$ | kcal/mol |
| 14 | $CCC(L, K)$ | Pressure broadening coefficients for Kth band (see text for details) | 7F10.5 | $L = 1, \dots, 126$ $K = 1, \dots, 10$ | $\text{cm}^{-1} \text{atm}^{-1}$ |
| 15 | $FB(J, K)$ | Foreign-gas broadened linewidth of transition ($v+1, J-1 \rightarrow v, J$) by species K , $K = \text{H}_2, \text{N}_2, \text{F}_2, \text{Ar}, \text{He}, \text{H}, \text{F}$, and SF_6 , at 300 K | 5F16.5 | $J = 1, \dots, 15$ $K = 1, \dots, 8$ | $\text{cm}^{-1} \text{atm}^{-1}$ |

^aTAPE 8(9) contains the $CV_i(T)[EHPY_i(T)]$ arrays of the species in the order listed above.

Anderson theory for pressure broadening. The array is dimensioned CCC(126, 10), representing sets of 126 coefficients for each of 10 vibrational bands. These bands are: HF(0 - 1), HF(1 - 2), HF(2 - 3), HF(3 - 4), HF(4 - 5), DF(0 - 1), DF(1 - 2), DF(2 - 3), DF(3 - 4), and DF(4 - 5). Each set of 126 coefficients is additionally partitioned by means of an EQUIVALENCE statement into an array of the form C(7, 6, 3). The first index represents the seven coefficients needed for the equation

$$\begin{aligned} \gamma(m) = & c_1 + c_2 e^{-m/4} + c_3 m e^{-m/4} + c_4 m^2 e^{-m/2} \\ & + c_5 m e^{-m^2/8} + c_6 m^2 e^{-m^2/16} + c_7 e^{-m^2/8} \end{aligned} \quad (31)$$

which is the expression used by Meredith to represent the results of his Anderson theory calculation. In Eq. (31), m corresponds to the rotational quantum number for the lower level of the transition and $\gamma(m)$ is the Lorentz half linewidth at half maximum ($\text{cm}^{-1} \text{atm}^{-1}$). The coefficients c_i depend on the nature of the perturbing species, as well as on the gas temperature. The second index of array C(7, 6, 3) designates six different possible perturbers: HF(0), HF(1), HF(2), DF(0), LF(1), and DF(2). The third index represents the three temperatures for which the coefficients are given: 300, 600, and 900 K. For calculations of linewidth at temperatures other than these, linear interpolations and extrapolations are presently used.

The foreign-gas pressure broadening coefficients stored in the array FB(15, 8) correspond to the fifteen vibrational-rotational transitions modeled for each band and eight possible perturbing molecules: H_2 , N_2 , F_2 , Ar, He, H, F, and SF_6 . These coefficients were obtained experimentally at sample gas temperatures of ~ 300 K. At higher temperatures, a $\gamma(m) \sim T^{1/2}$ dependence is assumed for the present calculations, based on a hard sphere interaction model (Ref. 1).

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APPENDIX A

RATE COEFFICIENTS FOR $H_2 + F_2$ CHEMICAL LASER

The chemical kinetic model used for the rate-equation solution has been suggested by Cohen (Ref. 4) and is shown in Table A-1. Rate coefficients k and k_* designate forward and backward rates, respectively. For each reaction, the missing rate coefficient is determined from the equilibrium constant.

Table A-1. Rate Coefficients for $H_2 + F_2$ Chemical Laser^a

| Reaction No. | Reaction | Rate Coefficient, $cm^3 \text{ mol}^{-1} \text{ sec}^{-1}$ | M, v |
|--------------|-------------------------------|---|-----------------------------------|
| 11 | $F + H_2(0) = HF(1) + H$ | $k_{11} = 2.6 \times 10^{13-1.6/\theta}$ | |
| 12 | $F + H_2(0) = HF(2) + H$ | $k_{12} = 8.8 \times 10^{13-1.6/\theta}$ | |
| 13 | $F + H_2(0) = HF(3) + H$ | $k_{13} = 4.4 \times 10^{13-1.6/\theta}$ | |
| 14 | $F + H_2(0) = HF(4) + H$ | $k_{14} = 7.4 \times 10^{12-0.50/\theta}$ | |
| 15 | $F + H_2(0) = HF(5) + H$ | $k_{15} = 1.1 \times 10^{13-0.51/\theta}$ | |
| 16 | $F + H_2(0) = HF(6) + H$ | $k_{16} = 1.9 \times 10^{13-0.56/\theta}$ | |
| 17 | $H + F_2 = HF(0) + F$ | $k_{17} = 1.1 \times 10^{12-2.4/\theta}$ | |
| 18 | $H + F_2 = HF(1) + F$ | $k_{18} = 2.5 \times 10^{12-2.4/\theta}$ | |
| 19 | $H + F_2 = HF(2) + F$ | $k_{19} = 3.5 \times 10^{12-2.4/\theta}$ | |
| 20 | $H + F_2 = HF(3) + F$ | $k_{20} = 3.6 \times 10^{12-2.4/\theta}$ | |
| 21 | $H + F_2 = HF(4) + F$ | $k_{21} = 1.6 \times 10^{13-2.4/\theta}$ | |
| 22 | $H + F_2 = HF(5) + F$ | $k_{22} = 3.6 \times 10^{13-2.4/\theta}$ | |
| 23 | $H + F_2 = HF(6) + F$ | $k_{23} = 4.8 \times 10^{13-2.4/\theta}$ | |
| 24 | $H + F_2 = HF(7) + F$ | $k_{24} = 5.5 \times 10^{12-2.4/\theta}$ | |
| 25 | $H + F_2 = HF(8) + F$ | $k_{25} = 2.5 \times 10^{12-2.4/\theta}$ | |
| 26-41 | $HF(v) + M_1 = HF(v') + M_1$ | $k_{26-41} = v^{1.3} 10^{14.0} T^{-0.8} + 10^{0.4} T^{3.5}$ | $M_1 = HF, v = 1 \dots 8, v' < v$ |
| 42 | $HF(1) + M_2 = HF(0) + M_2$ | $k_{42} = 1.5 \times 10^{10-1.1/\theta} T$ | $M_2 = F$ |
| 43 | $HF(2) + M_2 = HF(1) + M_2$ | $k_{43} = 1.5 \times 10^{10-0.5/\theta} T$ | |
| 44-49 | $HF(v) + M_2 = HF(v-1) + M_2$ | $k_{44-49} = 1.5 \times 10^{10} T$ | $v = 3 \dots 8$ |
| 50-57 | $HF(v) + M_4 = HF(v-1) + M_4$ | $k_{50-57} = (8 \times 10^{-4} T)^{1/2}$ | $M_4 = Ar, F_2; v = 1 \dots$ |

Table A-1. Rate Coefficients for $H_2 + F_2$ Chemical Laser^a (Continued)

| Reaction No. | Reaction | Rate Coefficient, cm ³ mol ⁻¹ sec ⁻¹ | M, v |
|--------------|---------------------------------------|---|--|
| 58-93 | $HF(v) + M_6 = HF(v') + M_6$ | $k_{58-93} = 1.8 \times 10^{13-0.7/T}$ | $M_6 = H, v = 1 \dots 8, v' < v$ |
| 94-101 | $HF(v) + M_5 = HF(v-1) + M_5$ | $k_{94-101} = v(8.7 \times 10^{-7} T^5)$ | $M_5 = He, v = 1 \dots 8$ |
| 102-109 | $HF(v) + M_7 = HF(v-1) + M_7$ | $k_{102-109} = v(1 \times 10^5 T^2)$ | $M_7 = H_2, v = 1 \dots 8$ |
| 110-116 | $HF(v) + HF(v) = HF(v-1) + HF(v+1)$ | $k_{110-116} = 1.5 \times 10^{12} T^{1/2}$ | $v = 1 \dots 7$ |
| 118-123 | $HF(v) + HF(v+1) = HF(v-1) + HF(v+2)$ | $k_{118-123} = 0.5k_{4a}$ | $v = 1 \dots 6$ |
| 125-129 | $HF(v) + HF(v+2) = HF(v-1) + HF(v+3)$ | $k_{125-129} = 0.25k_{4a}$ | $v = 1 \dots 5$ |
| 131-134 | $HF(v) + HF(v+3) = HF(v-1) + HF(v+4)$ | $k_{131-134} = 0.125k_{4a}$ | $v = 1 \dots 4$ |
| 135 | $HF(0) + H_2(1) = HF(1) + H_2(0)$ | $k_{135} \approx 9 \times 10^{11}$ | |
| 136 | $HF(1) + H_2(1) = HF(2) + H_2(0)$ | $k_{136} \approx 2.9 \times 10^{12}$ | |
| 137 | $HF(2) + H_2(1) = HF(3) + H_2(0)$ | $k_{137} \approx 9 \times 10^{12}$ | |
| 138 | $HF(3) + H_2(1) = HF(4) + H_2(0)$ | $k_{138} \approx 2 \times 10^{13}$ | |
| 139 | $HF(0) + H_2(2) = HF(1) + H_2(1)$ | $k_{139} = k_{5a}$ | |
| 140 | $HF(1) + H_2(2) = HF(2) + H_2(1)$ | $k_{140} = k_{5b}$ | |
| 141-142 | $H_2(v) + M_8 = H_2(v-1) + M_8$ | $k_{141-142} = v(2.5 \times 10^{-4} T^{4.3})$ | $v = 1, 2, M_8 = \text{all except H, H}_2$ |
| | $H_2(v) + M_9 = H_2(v-1) + M_9$ | $k_{141-142} = v(10^{-3} T^{4.3})$ | $v = 1, 2, M_9 = H, H_2$ |
| 143-150 | $HF(v) + M_{11} = HF(v-1) + M_{11}$ | $k_{143-150} = v^{2.5} (11 T^3 + 2.4 \times 10^9)$ | $v = 1, \dots, 8$ $M_{11} = N_2, SF_6$ |

^aNote that dissociation-recombination reactions have been neglected.

^b $\theta = 4,575$ T/1000 kcal/mol

^cv = vibrational level; M = collision partner

APPENDIX B

FLASH-LAMP FORMULATION FOR OPTICALLY THIN GASES

For an optically thin gas mixture, the approximation

$$\exp(-Z_2 n_{F_2}) \cong 1 - Z_2 n_{F_2} \quad (B-1)$$

can be made. Thus, Eq. (29) can be written

$$\left(\frac{dn_{F_2}}{dt} \right)_{fl} \cong - Z_1 Z_2 n_{F_2} I(t) \quad (B-2)$$

Since two F atoms are introduced for every F_2 dissociated,

$$\left(\frac{dn_F}{dt} \right)_{fl} \cong 2 Z_1 Z_2 n_{F_2} I(t) \quad (B-3)$$

For low initiation levels, e.g., $F/F_2 \leq 2\%$, Eq. (B-3) can be integrated to obtain

$$\frac{[F]}{[F_2]} \cong 2 Z_1 Z_2 \int I(t) dt \quad (B-4)$$

where the notation $[F_2]$ was substituted for n_{F_2} . With a normalized intensity profile assumed, i.e.,

$$\int I(t) dt = 1 \quad (B-5)$$

$$\frac{[F]}{[F_2]} \approx 2 Z_1 Z_2 \quad (B-6)$$

is obtained. Thus, the quantity $2 Z_1 Z_2$ is approximately the initiation level of the laser, and can be empirically set to the measured experimental value.

APPENDIX C

LISTING FOR MODEL SPIKE

PRC(OM SPIKEWF

CC.....FOREIGN GAS LINE PROTECTING PARAMETERS

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PROGRAM SPIKEMF

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55 C.....HEAT CAPACITY
C.....READ(8,51) CVF,CVF2,CVN2,CVSF6,CVM2,CVMF,CVC,CV02,CV0H,CVM20,CVM02
C.....ENTHALPY OF GASES
C.....READ(9,49) EMPY1,EMPY2,EPYF,EPYF2,EMPYH,EPY0,EPY02,EMPYCH,
1 EMPYH20,EPYH2
C.....LINE WIDTH PARAMETERS,CCC ARE SELF-BROADENING COEFFICIENTS
C.....DEFINITION, F2 AND F20LC ARE EXPERIMENTAL FOREIGN GAS
C.....BROADENING LINE WIDTHS. UNITS: 1/CM*ATM
C.....READ(10,53) CCC
C.....CALL INPUT1
C.....TRY REDUCING F2 BROADENING COEFFICIENT
C.....F23C=1.
C.....DO 1 J=1,15
C.....FRI(J,3)=F2(J,3)/F23C
C.....CONVERTS GAS FRACTIONS TO MOLE/CC
C.....FCIR=.5348E-7*PRESS*(300./TEMP)
C.....INTEGRATION PARAMETERS FOR DIFSUB
C.....DELIM=1.E-15
C.....ALIM=DELIM/100.
C.....MAXDEP=9
C.....NFC=150
C.....MF=0
C.....KKK=0
C.....TSTEP=1SKIP
C.....NC=0
C.....JCNT IS NC. STEPS BETWEEN. CHECK FOR J-SHIFTS
C.....JCNT=1
C.....JGAIN=JCNT
C.....LASER POWER,PULSE ENERGY, ENERGY FOR EACH BAND:
C.....POWER=0.
C.....ENGY=0.
C.....PL=0.
C.....T=0.
C.....PULAS=0.
C.....DO 2 I=1,3
C.....JMAX(I)=4

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PROGRAM SPIKEHF

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110 C.....POWER,ENERGY,GAIN, FOR EACH LINE(TRANSITION), P(I,J)
C
C DO 2 J=1,150
C   I=J*(J+1)/2
C   E(I,J)=0.
C   ALPH(I,J)=0.
C   DO 3 I=1,NVAR
C     Y(I,I)=1.E-6
C     YMAX(I)=1.E-6
C
C.....RCIF(I) IS FORWARD RATE OF REACT I, RCIF(I) IS BACKWARD
C.....RATE OF REACT I, SF IS NET FORWARD RATE
C
C 4 I=1,186
C   RCIF(I)=0.
C   SF(I)=0.
C
C.....DILUENT SPECIES CONCENTRATIONS, MOLES/CC
C
C ME=RH*FCTR
C NZ=RN2*FCTR
C SF6=YSF6*FCTR
C AR=AR*FCTR
C
C.....INITIAL VALUES Y(I,N)
C.....HF(V) CONCENTRATION, V = N - 1
C.....UNDEFINED, RESEPCION FOR ACO. VAR.
C.....H-ATOM CONCENTRATION
C.....H2(V) CONCENTRATION V = N - 10
C.....F-ATOM CONCENTRATION
C.....F2 CONCENTRATION
C.....TRANSLATIONAL TEMPERATURE
C.....PHOTON FLUX, F(V,N)
C
C Y(1,1)=RH*FCTR
C Y(1,16)=R02*FCTR
C Y(1,17)=H1*FCTR
C Y(1,18)=H2*FCTR
C Y(1,19)=F1*FCTR
C Y(1,20)=F2*FCTR
C Y(1,21)=TEMP
C Y(1,22)=T
C Y(1,1)=FLUX
C
C.....CHECK TEMPERATURE AND READ CORRESPONDING
C.....COEFFICIENTS
C.....AND BACKWARD(RGR) RATE
C
C KT=UY(1,23)-100.)/25.*1.5
C CO 5 I=1,KT

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160 BEAT (12.50) *KF
161 READ (7.20) A
162 IF (A2.0) A CALL RATE (Y(1.23))
163 IF (SE6.0) A CALL RATE (Y(1.23))
164 IF (SE6.0) A CALL RATE (Y(1.23))
165
166 .....INTEGRATION LOOP
167
168 TOL=1
169 IF (1.0) GO TO 12
170
171 .....FLASHLAMP INTENSITY CONTAINED VIA INTERPOLATION
172 .....OF FLASHLAMP Pz(FILE
173
174 KF=0
175 DO 4 I=1,20
176   TEL=FLASH(2,I)
177   IF (TEL) KF=KF+1
178   IF (TEL) GO TO 4
179   CONTINUE
180   PFLASH=FLASH(1,KF)+(TEL/SH(2,KF))*(FLASH(1,KF+1)-FLASH(1,
181   ASH(2,KF+1)-FLASH(2,KF))
182   PFLASH=PFLASH*Z1*(1.-EXP(-Z2*Y(1.22)))
183   CONTINUE
184
185 .....CHECK TEMP. AND INPUT NEW RATE COEFFS. IF NEEDED.
186
187 AKI=(Y(1.23)-100.)/25.*1.5
188 IK=IFX(AIKT)
189 IF (IK) GO TO 12
190 IF (IK) GO TO 12
191 IF (IK) GO TO 12
192 IF (IK) GO TO 12
193 IF (IK) GO TO 12
194 IF (IK) GO TO 12
195
196 .....COMPUTE RATE COEFFS. CORRESPONDING TO K2 OR
197 .....SF6 DEACTIVATION.
198
199 IF (IN2.0) CALL RATE (Y(1.23))
200 IF (SE6.0) CALL RATE (Y(1.23))
201 IF (SE6.0) CALL RATE (Y(1.23))
202
203 .....UPDATE SELF-RRACENEO LINEMIDTH
204
205 IF (TEL) GO TO 500
206 PMOL(1)=Y(1.1)
207 PMOL(2)=Y(1.2)
208 PMOL(3)=Y(1.3)+Y(1.4)+Y(1.5)+Y(1.6)+Y(1.7)+Y(1.8)+Y(1.9)

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PROGRAM SPIKEHF

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215      CALL LORENTZ (Y(1,23),15)
      C.....CHECK FOR J-SHIFT IF NO. OF STEPS SINCE
      C.....LAST CHECK(JGAIN) IS .GE. JCMT
      C
      JGAIN=JGAIN+1
      YF (JGAIN-JCMT) 14,16,16
220      C.....COMPUTE GAIN FOR THE LINES NEAR J-MAX ONLY, THEN
      C.....PROCEED TO INTEGRATION
      C
      DO 15 I=1,8
      IV=I-1
      JLOW=JMAX(I)-3
      JHIGH=JMAX(I)+3
      DO 15 J=JLOW,JHIGH
      ALPHA(I,J)=GAINC2(IV,J,79,Y)
      GO TO 29
225      C.....COMPUTE GAIN FOR EACH POSSIBLE TRANSITION TO LOWER LEVEL (IV,J)
      C.....TO CHECK FOR J-SHIFT
      C
      JGAIN=0
      DO 17 I=1,8
      IV=I-1
      DO 17 J=1,15
      ALPHA(I,J)=GAINC2(IV,J,79,Y)
230      C.....CHECK J-SHIFT
      C.....DETERMINE THE J (LOWER LEVEL) OF MAX GAIN
      C
      DO 28 I=1,8
      JMAXO=JMAX(I)
      JMAX(I)=4
      JM=4
      DO 18 J=5,13
      IF (ALPHA(I,J).LE.ALPHA(I,JM)) GO TO 18
      JMAX(I)=J
      JM=J
      CONTINUE
      IF (JMAX(I).EQ.4) GO TO 19
      CONTINUE
      IF (JMAX(I).EQ.JMAXO) GO TO 28
235      C.....IF A J-SHIFT HAS OCCURRED, REDEFINE THE APPROPRIATE F(V,J) AND
      C.....REINITIALIZE
      C.....THE Y(I,N) CORRESPONDING TO PHOTON FLUXES ARE
      C.....REDEFINED TO REPRESENT NEW TRANSITIONS IN EACH BAND
      C
      JSTART=0
      LJ=JMAX(I)-JMAXO
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255
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12/21/77

PROGRAM SPIKEHF

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270      L=7*I+16
        IF (LJ,LT,0) GO TO 22
        IF (LJ,GE,7) GO TO 26
        KS=7-LJ
        DO 20 M=1,KS
          Y(1,L+M)=Y(1,L+LJ+M)
        CO 21 N=1,LJ
          Y(1,L+N+KS)=FLUX
        GO TO 28
275      NLJ=LJ
        IF (NLJ,GE,7) GO TO 26
        NKS=7-NLJ
        DO 23 M=1,NKS
          STORE(M)=Y(1,L+M)
        CO 24 M=1,NKS
          Y(1,L+NLJ+M)=STORE(M)
        DO 25 M=1,NLJ
          Y(1,L+M)=FLUX
        GO TO 28
285      DO 27 M=1,7
          Y(1,L+M)=FLUX
        CONTINUE
        .....INTEGRATE
290      CALL DISUB (INVAR,T,Y,SAVE,M,HV1P,HVAP,EPS,MF,YMAX,EOROR,KFLAG,JST
        INCT=INCT+1
        GO TO 31
295      .....RETRY LAST STEP WITH SMALLER STEP SIZE
        H=HMIN
        HMT=HMIN/20.
        JST=JST+1
        GO TO 29
300      CONTINUE
305      .....IF INTEGRATION UNSUCCESSFUL, GO TO 45
        IF (KFLAG,LE,0) GO TO 45
310      .....MAINTAIN MINIMUM PHOTON FLUXES AT *NOISE LEVEL*
        DO 32 I=24,79
          IF (Y(1,I).LT,FLUX) Y(1,I)=FLUX
        CONTINUE
315      .....COMPUTE LASER PULSE POWER(PPOWER) AND PULSE ENERGY(ENGY).
        .....PLANE AND ELINE CORRESPOND TO POWER AND ENERGY FOR EACH
        .....TRANSITION. H1 = STEP SIZE CONST = CCONVERSI* FACTOR
        H1=T-TOLC

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PROGRAM SPIKEHF

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320 CONST=2.85912*THGAIN
    CONST=CONST*USPOWER
    POWER=0.
    DO 33 I=1,8
    K=JMAX(I)-4
    L=7+I+16
    DO 33 J=L,7
    Y(I,L+J)=Y(I,L+J)+C(I,K+J)*CONST*4.184
    PLINE(I,K+J)=POWER+PLINE(I,K+J)
    POWER=POWER+PLINE(I,K+J)
    PLINE(I,K+J)=ELINE(I,K+J)+PLINE(I,K+J)*H1
    ENG=ENG+POWER*H1
33
C.....CHECK FOR PULSE TERMINATION, PRINT STEP AND QUICK LOOK
C.....OPTION (PRINTAL PRINT)
    IF (I.GT.1) I=1
    IF (I.LT.16) GO TO 500
    IF (I.LT.16) GO TO 44
    IF (I.LT.16) SKIP
    IF (I.LT.16) GO TO 41
C.....OUTPUT COMMANDS
500 CONTINUE
    PRINT 1, I, RUNNUM
    PRINT 1, I, RUN NO, SFF - *.13, //
    PRINT 5, I, S, I, 2, NCT, I, 1
    PRINT 5, I, POWER, ENG
    PRINT 5, I, Y(I,17), Y(I,21), Y(I,22), Y(I,13), Y(I,13), Y(I,20)
    PRINT 6, I, (Y(I,1), I=1, 5)
    PRINT 6, I, Y(I,15), Y(I,16), (Y(I,1), I=60, 93), N2, SFF5
    PRINT 6, I, T, 2) GO TO 41
    PRINT 6, I, I=1, 8
    IV=I-1
    PRINT 1, I, IV, JMAX(I), (Y(I,L+J), J=1, 7)
    CONTINUE
    DO 36 I=1, 8
    K=JMAX(I)-4
    IV=I-1
    PRINT 6, I, IV, JMAX(I), (ELINE(I,K+J), J=1, 7)
    CONTINUE
    PRINT 6, I, J=1, 15
    PRINT 7, I, J, (ELINE(I, J), I=1, 8)
    CONTINUE
37

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375 IF (X5,LT,3) GO TO 41
380 PRINT 39
385 GO TO 41
390 J=1,5
395 J, (ALPHA(I,J),I=1,8)
400 CONTINUE
405 LT,4) GO TO 41
410 PRINT 46
415 GO TO 46
420 J=1,5
425 J, (GAMMA(I,J),I=1,8)
430 CONTINUE
435 LT,5) GO TO 41
440 PRINT 47
445 GO TO 47
450 J=1,50
455 J, (E(I,J),I=1,8)
460 IF (K,0,1,86) GO TO 41
465 K=3, K,KFR(K),KRR(K),KOTF(K),RCTB(K),RF(K)
470 CONTINUE
475 CONTINUE
480 *****WRITE CUTOUT TO TAPE 13
485 GO 42 I=1,23
490 XXX(I)=V(1,I)
495 XXX(24)=T
500 XXX(25)=POWER
505 XXX(26)=ENGY
510 GO 43 I=1,3
515 GO 43 I=1,3
520 HMM=26, (I=1,3)*15,J
525 NMM=14, (I=1,3)*12,J
530 XXX(MV)=P, (I=1,3)*11,J
535 XXX(MV)=ALL, (I=1,3)*10,J
540 WRITE (13,*) XXX
545 KXX=KXX+1
550 *****CHECK FOR TERMINATION. IF NCT, RETURN TO 39
555 *****INTEGRATION LCCT(7)
560 GO TO 39
565 IF (T EQ,0.) GO TO 29
570 JSTART,1
575 IF (T,LE,TIME) GO TO 7
580 GO TO 16
585 *****INTEGRATION STEP WAS UNSUCCESSFUL. DETERMINE
590 *****TO TRY AGAIN WITH SMALLER STEP OR TO TERMINATE
595 IF (HMIN-GE,ALIM) GO TO 30
600 PRINT 75, KLAGT
605 CALL DIFFUN (T,Y,DERV1)
610 PRINT 76, JERV1

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1  SUBROUTINE FLOW (N, N1, N2, N3, N4, N5, N6, N7, N8, N9, N10, N11, N12, N13, N14, N15, N16, N17, N18, N19, N20, N21, N22, N23, N24, N25, N26, N27, N28, N29, N30, N31, N32, N33, N34, N35, N36, N37, N38, N39, N40, N41, N42, N43, N44, N45, N46, N47, N48, N49, N50, N51, N52, N53, N54, N55, N56, N57, N58, N59, N60, N61, N62, N63, N64, N65, N66, N67, N68, N69, N70, N71, N72, N73, N74, N75, N76, N77, N78, N79, N80, N81, N82, N83, N84, N85, N86, N87, N88, N89, N90, N91, N92, N93, N94, N95, N96, N97, N98, N99, N100, N101, N102, N103, N104, N105, N106, N107, N108, N109, N110, N111, N112, N113, N114, N115, N116, N117, N118, N119, N120, N121, N122, N123, N124, N125, N126, N127, N128, N129, N130, N131, N132, N133, N134, N135, N136, N137, N138, N139, N140, N141, N142, N143, N144, N145, N146, N147, N148, N149, N150, N151, N152, N153, N154, N155, N156, N157, N158, N159, N160, N161, N162, N163, N164, N165, N166, N167, N168, N169, N170, N171, N172, N173, N174, N175, N176, N177, N178, N179, N180, N181, N182, N183, N184, N185, N186, N187, N188, N189, N190, N191, N192, N193, N194, N195, N196, N197, N198, N199, N200, N201, N202, N203, N204, N205, N206, N207, N208, N209, N210, N211, N212, N213, N214, N215, N216, N217, N218, N219, N220, N221, N222, N223, N224, N225, N226, N227, N228, N229, N230, N231, N232, N233, N234, N235, N236, N237, N238, N239, N240, N241, N242, N243, N244, N245, N246, N247, N248, N249, N250, N251, N252, N253, N254, N255, N256, N257, N258, N259, N260, N261, N262, N263, N264, N265, N266, N267, N268, N269, N270, N271, N272, N273, N274, N275, N276, N277, N278, N279, N280, N281, N282, N283, N284, N285, N286, N287, N288, N289, N290, N291, N292, N293, N294, N295, N296, N297, N298, N299, N300, N301, N302, N303, N304, N305, N306, N307, N308, N309, N310, N311, N312, N313, N314, N315, N316, N317, N318, N319, N320, N321, N322, N323, N324, N325, N326, N327, N328, N329, N330, N331, N332, N333, N334, N335, N336, N337, N338, N339, N340, N341, N342, N343, N344, N345, N346, N347, N348, N349, N350, N351, N352, N353, N354, N355, N356, N357, N358, N359, N360, N361, N362, N363, N364, N365, N366, N367, N368, N369, N370, N371, N372, N373, N374, N375, N376, N377, N378, N379, N380, N381, N382, N383, N384, N385, N386, N387, N388, N389, N390, N391, N392, N393, N394, N395, N396, N397, N398, N399, N400, N401, N402, N403, N404, N405, N406, N407, N408, N409, N410, N411, N412, N413, N414, N415, N416, N417, N418, N419, N420, N421, N422, N423, N424, N425, N426, N427, N428, N429, N430, N431, N432, N433, N434, N435, N436, N437, N438, N439, N440, N441, N442, N443, N444, N445, N446, N447, N448, N449, N450, N451, N452, N453, N454, N455, N456, N457, N458, N459, N460, N461, N462, N463, N464, N465, N466, N467, N468, N469, N470, N471, N472, N473, N474, N475, N476, N477, N478, N479, N480, N481, N482, N483, N484, N485, N486, N487, N488, N489, N490, N491, N492, N493, N494, N495, N496, N497, N498, N499, N500, N501, N502, N503, N504, N505, N506, N507, N508, N509, N510, N511, N512, N513, N514, N515, N516, N517, N518, N519, N520, N521, N522, N523, N524, N525, N526, N527, N528, N529, N530, N531, N532, N533, N534, N535, N536, N537, N538, N539, N540, N541, N542, N543, N544, N545, N546, N547, N548, N549, N550, N551, N552, N553, N554, N555, N556, N557, N558, N559, N560, N561, N562, N563, N564, N565, N566, N567, N568, N569, N570, N571, N572, N573, N574, N575, N576, N577, N578, N579, N580, N581, N582, N583, N584, N585, N586, N587, N588, N589, N590, N591, N592, N593, N594, N595, N596, N597, N598, N599, N600, N601, N602, N603, N604, N605, N606, N607, N608, N609, N610, N611, N612, N613, N614, N615, N616, N617, N618, N619, N620, N621, N622, N623, N624, N625, N626, N627, N628, N629, N630, N631, N632, N633, N634, N635, N636, N637, N638, N639, N640, N641, N642, N643, N644, N645, N646, N647, N648, N649, N650, N651, N652, N653, N654, N655, N656, N657, N658, N659, N660, N661, N662, N663, N664, N665, N666, N667, N668, N669, N670, N671, N672, N673, N674, N675, N676, N677, N678, N679, N680, N681, N682, N683, N684, N685, N686, N687, N688, N689, N690, N691, N692, N693, N694, N695, N696, N697, N698, N699, N700, N701, N702, N703, N704, N705, N706, N707, N708, N709, N710, N711, N712, N713, N714, N715, N716, N717, N718, N719, N720, N721, N722, N723, N724, N725, N726, N727, N728, N729, N730, N731, N732, N733, N734, N735, N736, N737, N738, N739, N740, N741, N742, N743, N744, N745, N746, N747, N748, N749, N750, N751, N752, N753, N754, N755, N756, N757, N758, N759, N760, N761, N762, N763, N764, N765, N766, N767, N768, N769, N770, N771, N772, N773, N774, N775, N776, N777, N778, N779, N780, N781, N782, N783, N784, N785, N786, N787, N788, N789, N790, N791, N792, N793, N794, N795, N796, N797, N798, N799, N800, N801, N802, N803, N804, N805, N806, N807, N808, N809, N810, N811, N812, N813, N814, N815, N816, N817, N818, N819, N820, N821, N822, N823, N824, N825, N826, N827, N828, N829, N830, N831, N832, N833, N834, N835, N836, N837, N838, N
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1      FUNCTION GAINC2 (IV,J,N,Y)
2
3      THIS SUBROUTINE CALCULATES THE GAIN OF A P-BRANCH TRANSITION WITH
4      LOWER LEVEL ENERGY HF(I,J)
5      THIS SUBROUTINE TO BE USED WITH PROGRAM MODEL2.
6
7      DIMENSION Y(8,1,20)
8      COMMON /DEFUT/ SAVEL(100),SAVEI(12,100),ERROR(100),PH(1000)
9      COMMON /FAC/ F(10),G(9),H(8),I(7),O(9,61)
10     COMMON /CV/ CV(17),CVF(17),CVHF(17),CVSFE(17),CVN2(17)
11     COMMON /CVC/ CVC(17),CVC2(17),CVC3(17),CVC4(17),CVC5(17)
12     COMMON /CHV/ CHV(17),CHVF(17),CHVSFE(17),CHVN2(17),CHV3(17)
13     COMMON /EHPV/ EHPV(17),EHPVF(17),EHPVSFE(17),EHPVN2(17),EHPV3(17)
14     COMMON /EHPVC/ EHPVC(17),EHPVCF(17),EHPVCSFE(17),EHPVCN2(17),EHPVC3(17)
15     COMMON /NUNVAR/ NUNVAR,NFVAR,NFLAG,MEGAIN
16     COMMON /GAIN/ GAIN(8,15),THGAIN
17     COMMON /DETA/ DELT(17,13),HFV(17,13),FLUX,TAL(7,13),SIGNL(4)
18     COMMON /RAIR/ RAIR(186),VAR(186),RCT(186),RCT2(186),RF(196)
19     COMMON /ORAJEN/ ORAJEN,SPF6,AF,FE,N2
20     COMMON /POWER/ PL(18,15),ELINE(8,15),PL
21     COMMON /MISC/ LATTIC,MAX(8)
22     COMMON /BROAD/ COC(126,10),GAMMA(8,15),PMOL(6),FB(15,8)
23     REMAY=1,23
24     A1=TEM/100,*.5
25     I=IFIX(A1)
26
27     C.....A ARE CONSTANTS USED IN ERROR FCN APPROXIMATION
28
29     A=0.0705230784
30     A=0.0422932123
31     A=0.092705272
32     A=0.0015230143
33     A=0.002763672
34     A=0.000043063
35     WFE=2.00
36
37     .....DOFF AND LONTZ ARE DOFFLER AND LORENTZ LINEWIDTHS, RESPECT.
38     DOFF=3.581138E-7*WCI(IV+1,J)*SORT(TEM/WHF)
39
40     .....LORENTZ
41     GAMMA=SELF-BROADENING COEFF. COMPUTED IN SUBROUTINE
42
43     MSUM=(1,18)+Y(1,19)+Y(1,20)
44     LONTZ=.421+.7*MSUM/(TEM)+.1*P2
45     LONTZ=(J+1)+A*F(1,1)+.4*ME*F(J,5)+Y(1,17)*F8(J,6)+Y(1,21)*F(1,7)
46     Z=6*F8(J,6))+*(PMCL(1))+*(PMCL(2))+*(PMCL(3))+82.057*FE*GAMMA(IV+1,J)
47
48     .....COMPUTE VOIGT FUNCTION PER APPROX. OF ERROR FCN GIVEN
49     .....IN ABRAHAMOITZ AND STEGUN
50     YLINE=0.83255461*LONTZ/DOFF

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FUNCTION GAINC2

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55      IF (VLINE.GT.(2.4)) GO TO 1
      PHI=10.46971864/DOFF)*EXP(VLINE*VLINE)
      PHI=PHI*(1.+A1*VLINE+A2*VLINE**2+A3*VLINE**3+A4*VLINE**4+A5*VLINE**
      15+A6*VLINE**6))*(-16)
      GO TO 2
      CONST=2.*VLINE**2
      PHI=1.-CONST*(1.+3.*CONST*(-2)-15.*CONST*(-3)+105.*CONST*(-4
      1))/ (3.1415926535*CONT2)
      C..... COMPUTE POPULATIONS IN UPPER(NUP) AND LOWER(NLN) LEVELS.
      C..... ASSUMING BOLTZMANN DISTRIBUTION.
      2      NUP=(Y(1,IV+2)*(2.*FLOAT(J)-1.)/O(IV*2,IT*1))*EXP(-1.4387886*E(IV+
      12,J)/TEM)
      NLN=(Y(1,IV+1)*(2.*FLOAT(J)+1.)/O(IV*1,IT*1))*EXP(-1.4387886*E(IV+
      11,J+1)/TEM)
      C..... COMPUTE GAIN
      3      GAINC2=3.1753646E-11*MC(IV+1,J)*PHI*B(IV+1,J)*((2.*FLOAT(J)+1.)/
      12.FLOAT(J)-1.)*NUP*NLN
      GETURN
      ENC
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SUBROUTINE LORENTZ

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1  SUBROUTINE LORENTZ (T,M)
2  DIMENSION A(7), C(7,6,3), CC(126)
3  COMMON /BROAD/ CCC(126,10), GAMMA(6,15), PMOL(6), F9(15,8)
4  EQUIVALENCE (CC(1),C(1,1,1))
5
10 ..... THIS SUBROUTINE COMPUTES SELF-BROADENING COEFF. GAMMA
11 ..... FOR 800M HF AND CF MOLECULES. 126 COEFFICIENTS USED FOR EACH
12 ..... OF 10 BANDS, 5HF AND 5 CF. HF(0-1),..., HF(4-5), DF(0-1),...
13 ..... OF THE BANDS REPRESENTS SUCCESSIVELY THE 126 ELEMENTS IN EACH
14 ..... OF THE BANDS. CC INTS GROUPS CF 7 COEFFICIENTS, USED TO
15 ..... COMPUTE BROADENING BY EACH CF SPECIES. AT 3 TEMPERATURES
16 ..... KT IS USED TO INTERPOLATE/EXTRAPOLATE BETWEEN TEMPERATURES
17 ..... GAMMA= SELF-BROADENING COEFFICIENT, 1/CM-ATM
18
20 KT= IFIX(T/300.)
21 IF (T.LE.300.) KT=1
22 IF (T.GE.900.) KT=2
23
25 ..... PMOLSUM = TOTAL HF AND CF POPULATION
26 ..... PMOL(1) = HF(0)
27 ..... PMOL(2) = HF(1)
28 ..... PMOL(3) = HF(2,...,9)
29 ..... PMOL(4) = DF(0)
30 ..... PMOL(5) = DF(1)
31 ..... PMOL(6) = DF(2,...,10)
32
33 PMOLSUM=PMOL(1)+PMOL(2)+PMOL(3)+PMOL(4)+PMOL(5)+PMOL(6)
34 IF (PMOLSUM.LE.0.) GO TO 5
35 DO 3 IV=1,5
36 DO 1 I=1,126
37 CC(I)=CCC(I,IV)
38 DO 2 I=1,7
39 A(I)=1.
40 DO 2 J=1,5
41 C(I,J,KT)=C(I,J,KT+1)-C(I,J,KT)*KT/300.
42 A(I)=A(I)+C(I)*PMOL(J)/PMOLSUM
43 K=1
44 DO 4 K=1,6
45 X=A(I)*A(K)=A(I)*A(2)*EXP(-K/8.)+A(6)*A(2)*EXP(-K/16.)+A(7)*A(2)*EXP(-K/24.)
46 Y=1+X
47 GAMMA(I,K)=GAMMA(5,K)
48 GO TO 7
49 DO 6 I=1,8
50 DO 5 J=1,15
51 GAMMA(I,J)=0.
52 CONTINUE
53 RETURN
54 END

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SUBROUTINE DIFFUN
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SUBROUTINE DIFFUN

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SUBCUTINE DIFFUN

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SUPERCUTINE DIFFUN

The diagram illustrates a 1D lattice chain. The top part shows a chain of sites with various interactions: nearest-neighbor hopping (t), nearest-neighbor interaction (V), and next-nearest-neighbor interaction (V'). The bottom part shows a chain of sites with various interactions: nearest-neighbor hopping (t), nearest-neighbor interaction (V), and next-nearest-neighbor interaction (V'). The diagram is labeled with t , V , and V' .

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SUBROUTINE DIFFUN

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215      1RF(65)+RF(116)-VTMF(8)-VVHT(8)
C.....N2 V-T DEACTIVATION REACTIONS
C
DERVIV(1)=DERVIV(1)+PF(143)
DERVIV(9)=DERVIV(9)+PF(1150)
DO 20 I=1,6
DERVIV(I)=DERVIV(I)+RF(142+I)-RF(141+I)
20      C
C      NOW ADD MULTI-QUANTA (DELTA V .GT. 1) DEACTIVATION BY HF
C
RCTFMQ=0
DO 21 I=1,9
FX=0-FLQAT(I)
IF (I.GT.8) FX=0.
F2=1-LE(2) F2=0.
RCTFMQ=RCTFMQ+F2*(RCTF(36-I)+RCTF(44-I))
DERVIV(10-I)+RCTF(34-I)+RCTF(42-I))
DO 22 I=1,16
DERVIV(I)=0.
21      C
22      DERVIV(17)=COLD-HOT
DERVIV(18)=VTH2(1)-COLL
DERVIV(19)=VTH2(2)-VTH1(1)
DERVIV(20)=-VTH2(2)
C.....EFFECT OF FLASHLAMP ON F AND F2 CONCENTRATIONS.
C
DERVIV(21)=-DERVIV(17)+2.*PFLASH
DERVIV(22)=-HOT-PFLASH
PPHOTO=2.85912*WPHOTO+PFLASH
C.....OXYGEN KINETICS
C
DERVIV(15)=DERVIV(15)-2.*(RF(151)+RF(152))+RF(154)-RF(155)-RF(158)
1- RF(159)-RF(160)-RF(162)
DERVIV(16)=DERVIV(16)+RF(151)+RF(152)-RF(154)-RF(156)+RF(152)+RF(1
163)-RF(154)
DERVIV(17)+RF(153)-RF(154)+RF(155)-RF(156)-RF(157)-RF(1
158)-RF(161)-RF(162)
DERVIV(18)=DERVIV(18)-RF(153)-RF(155)+RF(162)
DERVIV(19)=DERVIV(19)-RF(153)-RF(154)+RF(155)-RF(157)+RF(158)-RF(1
159)+RF(161)+RF(162)
DERVIV(20)=DERVIV(20)+RF(153)+RF(154)+RF(155)+RF(157)+RF(160)
DERVIV(21)=DERVIV(21)+RF(153)+RF(154)+RF(155)+RF(157)+RF(160)
DERVIV(22)=DERVIV(22)+RF(153)+RF(154)+RF(155)+RF(157)+RF(160)
C      EFFECT OF RADIATION ON HF(V) CONCENTRATION
C      SIGNL(I) IS TOTAL RATE OF EMISSION FROM HF(I) TO HF(I-1)
C
DO 23 I=1,8
L=7*I+16
23      C
245      C
250      C
255      C
260      C
265      C

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[illegible]

SUBROUTINE DIFFUN

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SUBROUTINE DIFFS13

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SUBROUTINE QUESUB (N1,Y,SAVE,H,MIN,MMAX,EPS,MF,YMAX,ERROR,KFLAG,
1  N2,N3,N4,N5,N6,N7,N8,N9,N10,N11,N12,N13,N14,N15,N16,N17,N18,N19,N20,
5  N21,N22,N23,N24,N25,N26,N27,N28,N29,N30,N31,N32,N33,N34,N35,N36,N37,N38,
10 N39,N40,N41,N42,N43,N44,N45,N46,N47,N48,N49,N50,N51,N52,N53,N54,N55,N56,N57,N58,N59,N60,N61,N62,N63,N64,N65,N66,N67,N68,N69,N70,N71,N72,N73,N74,N75,N76,N77,N78,N79,N80,N81,N82,N83,N84,N85,N86,N87,N88,N89,N90,N91,N92,N93,N94,N95,N96,N97,N98,N99,N100)
10  KFLAG=1
15  IF (J1.EQ.1) GO TO 5
20  DO 2 J=1,N
25  SAVE(J,1)=Y(J,I)
30  IF (H.EQ.0) GO TO 4
35  IF (H.EQ.1) GO TO 7
40  IF (H.EQ.2) GO TO 10
45  IF (H.EQ.3) GO TO 13
50  IF (H.EQ.4) GO TO 16
55  IF (H.EQ.5) GO TO 19
60  IF (H.EQ.6) GO TO 22
65  IF (H.EQ.7) GO TO 25
70  IF (H.EQ.8) GO TO 28
75  IF (H.EQ.9) GO TO 31
80  IF (H.EQ.10) GO TO 34
85  IF (H.EQ.11) GO TO 37
90  IF (H.EQ.12) GO TO 40
95  IF (H.EQ.13) GO TO 43
100 IF (H.EQ.14) GO TO 46
105 IF (H.EQ.15) GO TO 49
110 IF (H.EQ.16) GO TO 52
115 IF (H.EQ.17) GO TO 55
120 IF (H.EQ.18) GO TO 58
125 IF (H.EQ.19) GO TO 61
130 IF (H.EQ.20) GO TO 64
135 IF (H.EQ.21) GO TO 67
140 IF (H.EQ.22) GO TO 70
145 IF (H.EQ.23) GO TO 73
150 IF (H.EQ.24) GO TO 76
155 IF (H.EQ.25) GO TO 79
160 IF (H.EQ.26) GO TO 82
165 IF (H.EQ.27) GO TO 85
170 IF (H.EQ.28) GO TO 88
175 IF (H.EQ.29) GO TO 91
180 IF (H.EQ.30) GO TO 94
185 IF (H.EQ.31) GO TO 97
190 IF (H.EQ.32) GO TO 100
195 IF (H.EQ.33) GO TO 103
200 IF (H.EQ.34) GO TO 106
205 IF (H.EQ.35) GO TO 109
210 IF (H.EQ.36) GO TO 112
215 IF (H.EQ.37) GO TO 115
220 IF (H.EQ.38) GO TO 118
225 IF (H.EQ.39) GO TO 121
230 IF (H.EQ.40) GO TO 124
235 IF (H.EQ.41) GO TO 127
240 IF (H.EQ.42) GO TO 130
245 IF (H.EQ.43) GO TO 133
250 IF (H.EQ.44) GO TO 136
255 IF (H.EQ.45) GO TO 139
260 IF (H.EQ.46) GO TO 142
265 IF (H.EQ.47) GO TO 145
270 IF (H.EQ.48) GO TO 148
275 IF (H.EQ.49) GO TO 151
280 IF (H.EQ.50) GO TO 154
285 IF (H.EQ.51) GO TO 157
290 IF (H.EQ.52) GO TO 160
295 IF (H.EQ.53) GO TO 163
300 IF (H.EQ.54) GO TO 166
305 IF (H.EQ.55) GO TO 169
310 IF (H.EQ.56) GO TO 172
315 IF (H.EQ.57) GO TO 175
320 IF (H.EQ.58) GO TO 178
325 IF (H.EQ.59) GO TO 181
330 IF (H.EQ.60) GO TO 184
335 IF (H.EQ.61) GO TO 187
340 IF (H.EQ.62) GO TO 190
345 IF (H.EQ.63) GO TO 193
350 IF (H.EQ.64) GO TO 196
355 IF (H.EQ.65) GO TO 199
360 IF (H.EQ.66) GO TO 202
365 IF (H.EQ.67) GO TO 205
370 IF (H.EQ.68) GO TO 208
375 IF (H.EQ.69) GO TO 211
380 IF (H.EQ.70) GO TO 214
385 IF (H.EQ.71) GO TO 217
390 IF (H.EQ.72) GO TO 220
395 IF (H.EQ.73) GO TO 223
400 IF (H.EQ.74) GO TO 226
405 IF (H.EQ.75) GO TO 229
410 IF (H.EQ.76) GO TO 232
415 IF (H.EQ.77) GO TO 235
420 IF (H.EQ.78) GO TO 238
425 IF (H.EQ.79) GO TO 241
430 IF (H.EQ.80) GO TO 244
435 IF (H.EQ.81) GO TO 247
440 IF (H.EQ.82) GO TO 250
445 IF (H.EQ.83) GO TO 253
450 IF (H.EQ.84) GO TO 256
455 IF (H.EQ.85) GO TO 259
460 IF (H.EQ.86) GO TO 262
465 IF (H.EQ.87) GO TO 265
470 IF (H.EQ.88) GO TO 268
475 IF (H.EQ.89) GO TO 271
480 IF (H.EQ.90) GO TO 274
485 IF (H.EQ.91) GO TO 277
490 IF (H.EQ.92) GO TO 280
495 IF (H.EQ.93) GO TO 283
500 IF (H.EQ.94) GO TO 286
505 IF (H.EQ.95) GO TO 289
510 IF (H.EQ.96) GO TO 292
515 IF (H.EQ.97) GO TO 295
520 IF (H.EQ.98) GO TO 298
525 IF (H.EQ.99) GO TO 301
530 IF (H.EQ.100) GO TO 304
535 IF (H.EQ.101) GO TO 307
540 IF (H.EQ.102) GO TO 310
545 IF (H.EQ.103) GO TO 313
550 IF (H.EQ.104) GO TO 316
555 IF (H.EQ.105) GO TO 319
560 IF (H.EQ.106) GO TO 322
565 IF (H.EQ.107) GO TO 325
570 IF (H.EQ.108) GO TO 328
575 IF (H.EQ.109) GO TO 331
580 IF (H.EQ.110) GO TO 334
585 IF (H.EQ.111) GO TO 337
590 IF (H.EQ.112) GO TO 340
595 IF (H.EQ.113) GO TO 343
600 IF (H.EQ.114) GO TO 346
605 IF (H.EQ.115) GO TO 349
610 IF (H.EQ.116) GO TO 352
615 IF (H.EQ.117) GO TO 355
620 IF (H.EQ.118) GO TO 358
625 IF (H.EQ.119) GO TO 361
630 IF (H.EQ.120) GO TO 364
635 IF (H.EQ.121) GO TO 367
640 IF (H.EQ.122) GO TO 370
645 IF (H.EQ.123) GO TO 373
650 IF (H.EQ.124) GO TO 376
655 IF (H.EQ.125) GO TO 379
660 IF (H.EQ.126) GO TO 382
665 IF (H.EQ.127) GO TO 385
670 IF (H.EQ.128) GO TO 388
675 IF (H.EQ.129) GO TO 391
680 IF (H.EQ.130) GO TO 394
685 IF (H.EQ.131) GO TO 397
690 IF (H.EQ.132) GO TO 400
695 IF (H.EQ.133) GO TO 403
700 IF (H.EQ.134) GO TO 406
705 IF (H.EQ.135) GO TO 409
710 IF (H.EQ.136) GO TO 412
715 IF (H.EQ.137) GO TO 415
720 IF (H.EQ.138) GO TO 418
725 IF (H.EQ.139) GO TO 421
730 IF (H.EQ.140) GO TO 424
735 IF (H.EQ.141) GO TO 427
740 IF (H.EQ.142) GO TO 430
745 IF (H.EQ.143) GO TO 433
750 IF (H.EQ.144) GO TO 436
755 IF (H.EQ.145) GO TO 439
760 IF (H.EQ.146) GO TO 442
765 IF (H.EQ.147) GO TO 445
770 IF (H.EQ.148) GO TO 448
775 IF (H.EQ.149) GO TO 451
780 IF (H.EQ.150) GO TO 454
785 IF (H.EQ.151) GO TO 457
790 IF (H.EQ.152) GO TO 460
795 IF (H.EQ.153) GO TO 463
800 IF (H.EQ.154) GO TO 466
805 IF (H.EQ.155) GO TO 469
810 IF (H.EQ.156) GO TO 472
815 IF (H.EQ.157) GO TO 475
820 IF (H.EQ.158) GO TO 478
825 IF (H.EQ.159) GO TO 481
830 IF (H.EQ.160) GO TO 484
835 IF (H.EQ.161) GO TO 487
840 IF (H.EQ.162) GO TO 490
845 IF (H.EQ.163) GO TO 493
850 IF (H.EQ.164) GO TO 496
855 IF (H.EQ.165) GO TO 499
860 IF (H.EQ.166) GO TO 502
865 IF (H.EQ.167) GO TO 505
870 IF (H.EQ.168) GO TO 508
875 IF (H.EQ.169) GO TO 511
880 IF (H.EQ.170) GO TO 514
885 IF (H.EQ.171) GO TO 517
890 IF (H.EQ.172) GO TO 520
895 IF (H.EQ.173) GO TO 523
900 IF (H.EQ.174) GO TO 526
905 IF (H.EQ.175) GO TO 529
910 IF (H.EQ.176) GO TO 532
915 IF (H.EQ.177) GO TO 535
920 IF (H.EQ.178) GO TO 538
925 IF (H.EQ.179) GO TO 541
930 IF (H.EQ.180) GO TO 544
935 IF (H.EQ.181) GO TO 547
940 IF (H.EQ.182) GO TO 550
945 IF (H.EQ.183) GO TO 553
950 IF (H.EQ.184) GO TO 556
955 IF (H.EQ.185) GO TO 559
960 IF (H.EQ.186) GO TO 562
965 IF (H.EQ.187) GO TO 565
970 IF (H.EQ.188) GO TO 568
975 IF (H.EQ.189) GO TO 571
980 IF (H.EQ.190) GO TO 574
985 IF (H.EQ.191) GO TO 577
990 IF (H.EQ.192) GO TO 
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SUBROUTINE DIFSUB

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SUBROUTINE DIFSUB

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215      50      RETURN
216      51      I=1,N
217      52      D=0+ERROR(I)/YMAX(I)**2
218      53      I=1,N
219      54      IF (D.GT.5) GO TO 55
220      55      IF (K.LT.3) GO TO 56
221      56      GO 52,J=3,K
222      57      I=1,N
223      58      V(I)=Y(I),I=1+(J)*ERROR(I)
224      59      KFLAG=+1
225      60      TIME=HOUR*LE.1) 50 TO 56
226      61      IDOUB=1000000
227      62      IDOUB=IDOUB*57.1) 50 TO 71
228      63      DO 54,I=1,N
229      64      SAVE(I)=1+ERROR(I)
230      65      GO TO 71
231      66      KFLAG=KFLAG-2
232      67      IF (KFLAG.LE.-1) GO TO 75
233      68      IF (KFLAG.LE.-1) GO TO 75
234      69      IF (KFLAG.LE.-1) GO TO 75
235      70      PR2=IDOUB*ENQ2*1.5
236      71      IF (PR2.LE.0) ENQ2=1.5
237      72      IF (IDOUB*MAXCER).OR.(KFLAG.LE.-1) GO TO 58
238      73      DO 57,I=1,N
239      74      D=0+((ERROR(I)-SAVE(I))/YMAX(I))**2
240      75      PR1=IDOUB*ENQ1*1.4
241      76      IF (PR1.LE.0) ENQ1=1.4
242      77      IF (IDOUB*LE.1) GO TO 60
243      78      DO 59,I=1,N
244      79      D=0+V(K(I))/YMAX(I)**2
245      80      PR1=IDOUB*ENQ1*1.3
246      81      CONTINUE
247      82      IF (PR2.LE.0) PR3=IDOUB*ENQ2*1.5
248      83      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
249      84      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
250      85      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
251      86      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
252      87      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
253      88      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
254      89      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
255      90      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
256      91      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
257      92      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
258      93      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
259      94      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
260      95      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
261      96      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
262      97      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
263      98      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
264      99      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5
265      100      IF (PR3.LE.0) PR3=IDOUB*ENQ2*1.5

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SUBROUTINE DIFSUB

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